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14. ABSTRACT
This report is intended to be a historical record of activities describing the research programs of the U.S. Army Research Laboratory - Army Research Office (ARL-ARO) for fiscal year 2017 (FY17; 1 Oct 2016 through 30 Sep 2017). This report provides: (i) an overview of the mission and strategy employed to guide ARO research investments and factors affecting the implementation of that strategy, (ii) a snapshot of end-of-year statistics of basic research funding (i.e., “6.1” funding) and program proposal activity, and (iii) research trends and key annual scientific discoveries and accomplishments of the ARO scientific divisions.

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ARO
IN REVIEW

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ARO in Review 2017

This document provides the annual historical record of the
U.S. Army Research Laboratory - Army Research Office (ARO) programs
for fiscal year 2017 (FY17), including program goals, management
strategies, funding information, and key accomplishments

Kelby O. Kizer, Ph.D.
Editor

ARO IN REVIEW 2017

TABLE OF CONTENTS

CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY

This report is intended to be a single-source document describing the research programs of the U.S. Army Research Office (ARO) for fiscal year 2017 (FY17; 1 Oct 2016 through 30 Sep 2017). This report provides:

- A brief review of the strategy employed to guide ARO research investments and noteworthy issues affecting the implementation of that strategy
- Statistics regarding basic research funding (*i.e.*, "6.1" funding) and program proposal activity
- Research trends and accomplishments of the individual ARO scientific divisions

I. ARO MISSION

The mission of ARO, as part of the U.S. Army Research Laboratory (ARL), is to execute the Army's extramural basic research program in the following disciplines: chemical sciences, computing sciences, electronics, life sciences (including social science), materials science, mathematical sciences, mechanical sciences, network sciences, and physics. The goal of this basic research is to drive scientific discoveries that will provide the Army with significant advances in operational capabilities through high-risk, high pay-off research opportunities, primarily with universities, but also with large and small businesses. ARO ensures that this research supports and drives the realization of future research relevant to all of the ARL Science and Technology (S&T) Campaigns, the ARL Essential Research Areas, and the Army Modernization Priorities. The results of these efforts are transitioned to the Army research and development community, industry, or academia for the pursuit of long-term technological advances for the Army.

II. ARO STRATEGY AND FUNCTION

ARO's mission represents the most long-range Army view for changes in its technology, with system applications often 20-30 years away. ARO pursues a long-range investment strategy designed to maintain the Army's overmatch capability in the expanding range of present and future operational capabilities. ARO competitively selects and funds basic research proposals from educational institutions, nonprofit organizations, and private industry. ARO executes its mission through conduct of an aggressive basic science research program on behalf of the Army to create cutting-edge scientific discoveries and the general store of scientific knowledge that is required to develop and improve weapons systems for land force dominance. The ARO research portfolio consists principally of extramural academic research efforts consisting of single investigator efforts, university-affiliated research centers, and specially tailored outreach programs. Each program has its own objectives and set of advantages as described further in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

ARL has eight S&T Campaigns (listed in Section III-B), including an extramural basic research campaign that ARO leads. ARL also pursues research in support of the Essential Research Areas (ERAs), which aim to address particular technology gaps for the current and future Army. ARO drives fundamental research efforts that will lead to new discoveries and increased understanding of the physical, engineering, and information sciences as they relate to long-term national security needs, in support of all of the ARL S&T Campaigns and ERAs.

The ARO strategy and programs, as part of the ARL Extramural Basic Research Campaign, are formulated in concert with the other ARL S&T Campaigns, the Research, Development and Engineering Command's (RDECOM's) Research, Development and Engineering Centers (RDECs), the Army Medical Research and Materiel Command (MRMC), the Army Corps of Engineers, and the Army Research Institute for the Behavioral and Social Sciences. ARO programs and research areas are intimately aligned with, and fully supportive of, the research priorities set within the DoD Quadrennial Defense Review, the DoD Strategic Basic Research Plan, the Army Modernization Priorities, the Assistant Secretary of Defense for Research and Engineering [ASD(R&E)] S&T Priorities, the Army S&T Master Plan, the Training and Doctrine Command (TRADOC) Army Capabilities Integration Center (ARCIC) Integrated S&T Lines of Effort, the TRADOC Army Warfighting Challenges, the Assistant Secretary of the Army for Acquisition, Logistics, and Technology [ASA(ALT)] Special Focus Areas, and the RDECOM Campaign Plan.

ARO serves the following functions in pursuit of its mission.

- Execute an integrated, balanced extramural basic research program
- Create and guide the discovery and application of novel scientific phenomena leading to leap-ahead technologies for the Army
- Drive the application of science to generate new or improved solutions to existing needs
- Accelerate research results transition to applications in all stages of the research and development cycle
- Strengthen the research infrastructures of academic, industrial, and nonprofit laboratories that support the Army
- Focus on research topics that support technologies vital to the Army's future force, combating terrorism and new emerging threats
- Leverage S&T of other defense and government laboratories, academia and industry, and organizations of our allies
- Foster training for scientists and engineers in the scientific disciplines critical to Army needs
- Actively seek creative approaches to enhance the diversity and capabilities of future U.S. research programs by enhancing education and research programs at historically black colleges and universities, and minority-serving institutions

III. IMPLEMENTING ARO STRATEGY

ARO employs multiple programs, initiatives, and investment strategies to fulfill its mission. A snapshot of the ARO research programs is provided in this section, and each program is described further in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

A. Program Snapshot

The research programs managed by ARO range from single investigator research to multidisciplinary/multi-investigator centers. A typical basic research grant within a program may provide funding for a few years, while in other programs, such as research centers affiliated with particular universities, a group of investigators may receive funding for many years to pursue novel research concepts. The programs for the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) are aimed at providing infrastructure and incentives to improve the diversity of U.S. basic research programs (see CHAPTER 2-IX). In addition to supporting the education of graduate students through basic research grants, the National Defense Science and Engineering Graduate (NDSEG) fellowship program is another mechanism through which ARO fosters the training of a highly-educated workforce skilled in DoD and Army-relevant research, which is critical for the future of the nation (see CHAPTER 2-X). ARO also has extensive programs in outreach to pre-graduate education to encourage and enable the next generation of scientists (see CHAPTER 2-XI). In addition, ARO guides the transition of basic research discoveries and advances to the appropriate applied-research and advanced-development organizations. ARO is actively engaged in speeding the transition of discovery into systems, in part through involvement in the development of topics and the management of projects in the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) programs (see CHAPTER 2-VIII).

B. Coordination for Program Development and Monitoring

The research programs and initiatives that compose ARO's extramural research program are formulated through ongoing and active collaborations throughout ARL, including the:

- ARL S&T Campaigns, in addition to the ARL Extramural Basic Research Campaign
  - Computational Sciences Campaign
  - Materials Research Campaign
  - Sciences-for-Maneuver Campaign
  - Information Sciences Campaign
  - Sciences for Lethality-and-Protection Campaign
  - Human Sciences Campaign
  - Assessment and Analysis Campaign
- ARL Essential Research Areas (ERAs), in addition to the Discovery ERA
  - Human Agent Teaming
  - Artificial Intelligence and Machine Learning
  - Cyber and Electromagnetic Technologies for Complex Environments
  - Distributed and Cooperative Engagement in Contested Environments
  - Tactical Unit Energy Independence
  - Manipulating Physics of Failure for Robust Performance of Materials
  - Science of Manufacturing at the Point of Need
  - Accelerated Learning for a Ready and Responsive Force
- ARL Directorates:
  - Computational and Information Sciences Directorate (ARL-CISD)
  - Human Research and Engineering Directorate (ARL-HRED)
  - Sensors and Electron Devices Directorate (ARL-SEDD)
  - Survivability/Lethality Analysis Directorate (ARL-SLAD)
  - Vehicle Technology Directorate (ARL-VTD)
  - Weapons and Materials Research Directorate (ARL-WMRD)

ARO programs are also formulated through collaborations with other Federal research organizations, including:

- RDECOM's RDECs
- Army Medical Research and Materiel Command (MRMC)
- Army Corps of Engineers (ACE)
- Army Research Institute for the Behavioral and Social Sciences
- Army Training and Doctrine Command (TRADOC)

ARO's extramural research program provides foundational discoveries in support of the ARL S&T Campaign Plan. While the ARL Directorates and the RDECOM Centers are the primary users of the results of the ARO research program, ARO also supports research of interest to ACE, MRMC, other Army Commands, and DoD agencies. Coordination and monitoring of the ARO extramural program by the ARL Directorates, RDECs, and other Army laboratories ensures a highly productive and cost-effective Army research effort. The University

Affiliated Research Centers (UARCs) and Multidisciplinary University Research Initiative (MURI) centers benefit from the expertise and guidance provided by the ARL Directorates, RDECs, and other DoD, academic, and industry representatives who serve on evaluation panels for each UARC.

The ARO-managed OSD research programs include the University Research Initiative (URI) programs, and the Research and Educational Program (REP) for HBCU/MSIs. These programs fall under the executive oversight of the Defense Basic Research Advisory Group. This group is led by the ASD(R&E) Director for Research, representatives from the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the Defense Advanced Research Projects Agency (DARPA), ARO, and ASAALT.

ARO programs are also developed and managed with a focus on supporting future Army needs as identified in the Army Modernization Priorities. These priorities were under development in FY17 and published in FY18, with details available at the Army's website.[1] These priorities emphasize a significant change in how the Army pursues solutions for the current and future warfighter. ARO's strategy is clearly aligned with the needs of the future warfighter, and supports all of the Army Modernization Priorities. As described earlier, ARO's mission represents the most long-range Army view for changes in its technology, with research focused on fundamental discoveries with system applications to ensure technological superiority 20-30 years away. ARO pursues a long-range investment strategy designed to maintain the Army's overmatch capability in the expanding range of present and future operational capabilities.

The Army Modernization Priorities are listed below. Refer to the Army's website for documentation detailing each of these priorities.

- Long-range Precision Fires
- Next-generation Combat Vehicle
- Future Vertical Lift
- Army Network
- Air and Missile Defense
- Soldier Lethality

IV. REVIEW AND EVALUATION

The ARO Directorates, Divisions, and Programs are evaluated by a wide range of internal (Army) and external (Academic, other Government) reviews, such as the former biennial ARO Division Reviews and the upcoming Technical Assessment Board (TAB) Review, beginning in FY18. For additional information regarding these review processes, the reader is encouraged to refer to the corresponding presentations and reports from each review (not included here).

[1] https://www.army.mil/e2/c/downloads/500971.pdf

V. ARO ORGANIZATIONAL STRUCTURE

The organizational structure of ARO mirrors the departmental structure found in many research universities. ARO's scientific divisions are aligned to a specific scientific discipline (*e.g.*, chemical sciences), and supported by the Operations Directorate (see FIGURE 1).

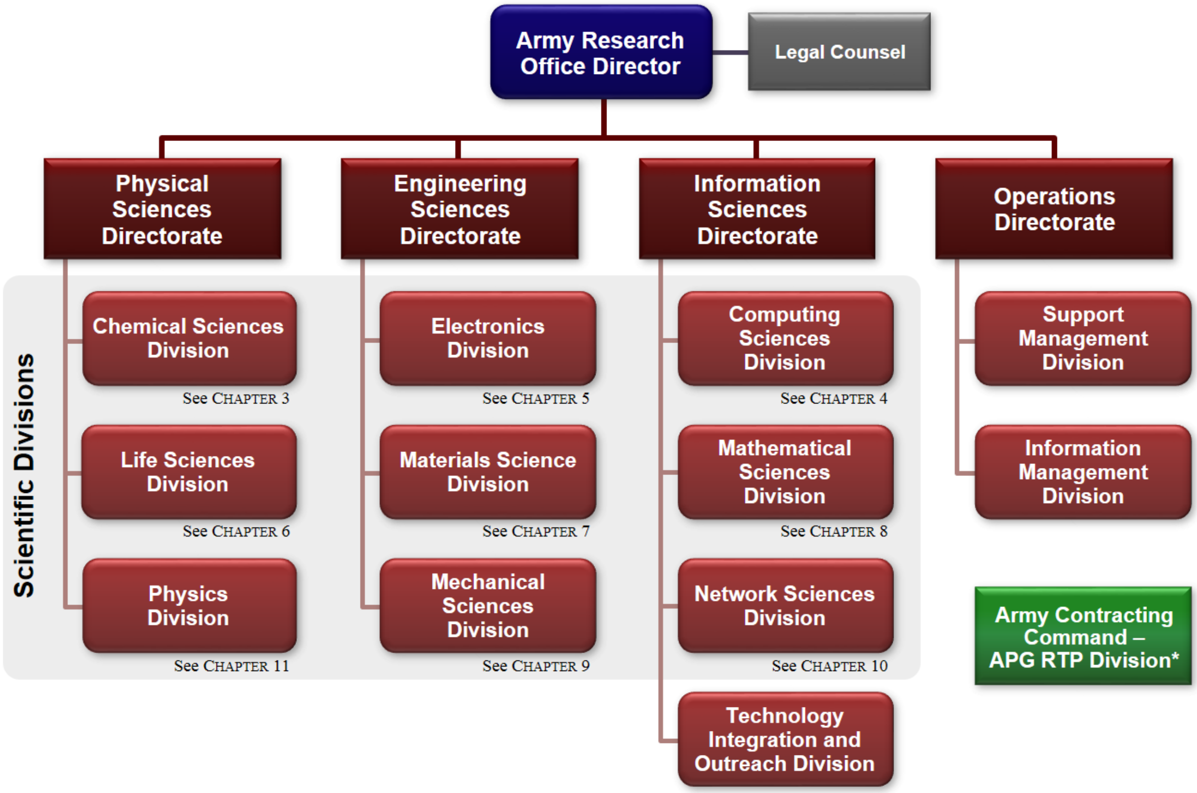

FIGURE 1

ARO Organizational Structure. ARO's scientific divisions fall under the Physical Sciences, Engineering Sciences, and Information Sciences Directorates. Each scientific Division has its own vision and research objectives, as described further in CHAPTERS 3-11. *Army Contracting Command – Army Proving Ground (APG), Research Triangle Park (RTP) Division executes the contracting needs for ARO-funded research; however, as part of the Army Contracting Command (*i.e.*, not ARL), it also performs contracting activities throughout RDECOM.

VI. ARO DIRECTOR'S OFFICE STAFF

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CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES

As described in the previous chapter, ARO pursues a variety of investment strategies to meet its mission as the Army's lead extramural basic research agency in chemical sciences, computing sciences, electronics, life sciences (including social science), materials science, mathematical sciences, mechanical sciences, network sciences, and physics. In this role, ARO serves as ARL's lead for the Extramural Basic Research Campaign (refer to CHAPTER 1 - Section III). ARO implements its investment strategies through research programs and initiatives that have unique objectives, eligibility requirements, and receive funding from a variety of DoD sources. The visions, objectives, and funding sources of these programs are presented in this chapter.

The selection of research topics, proposal evaluation, and project monitoring are organized within ARO Divisions according to scientific discipline (refer to the organizational chart presented in CHAPTER 1). ARO's Divisions are aligned with these disciplines, each with its own vision and research objectives, as detailed in CHAPTERS 3-11. Each Division identifies topics that are included in the broad agency announcement (BAA). Researchers are encouraged to submit white papers and proposals in areas that support the Division's objectives. The ARO Divisions are not confined to only funding research in the academic departments that align with the Division names; they have the flexibility to find and fund the most promising research to advance their mission regardless of the academic department pursuing a particular research idea.

I. OVERVIEW OF PROGRAM FUNDING SOURCES

ARO oversees and participates in the topic generation, proposal solicitation, evaluation, and grant-monitoring activities of programs funded through a variety of DoD agencies, as listed in the following subsections.

A. Army Funding

The Army funds the majority of the extramural basic research programs managed by ARO, as listed below.

- The Core (BH57) Research Program, funded through basic research "BH57" funds (see Section II).
- The University Research Initiative (URI), which includes these component programs:
  - Multidisciplinary University Research Initiative (MURI) program (see Section III)
  - Presidential Early Career Awards for Scientists and Engineers (PECASE; see Section IV)
  - Defense University Research Instrumentation Program (DURIP; see Section V)
- Three University Affiliated Research Centers (UARCs; see Section VI)

ARO coordinates with the Office of the Secretary of Defense (OSD) in managing the URI programs and also manages the Army's Small Business Technology Transfer (STTR) program (see Section VIII).

B. Office of the Secretary of Defense (OSD) Funding

The funds for a variety of programs managed or supported by ARO are provided by OSD.

- Research and Educational Program (REP) for Historically Black Colleges and Universities and Minority Serving Institutions (HBCU/MSI; see Section IX)
- National Defense Science and Engineering Graduate (NDSEG) Fellowships (see Section X)
- Youth Science Activities (see Section XI)

These activities are mandated by DoD's Chief Technology Office, the Assistant Secretary of Defense for Research and Engineering ASD(R&E). Each of these OSD-funded programs has a unique focus and/or a unique target audience. ARO has been designated by ASD(R&E) as the lead agency for the implementation of REP for HBCU/MSI activities on behalf of the three Services. OSD oversees ARO management of the Army-funded URI and its component programs (MURI, PECASE, and DURIP).

C. Other Funding Sources

In addition to the Army- and OSD-funded programs described earlier in this section, ARO leverages funds from other DoD sources (*e.g.*, Defense Advanced Research Projects Agency [DARPA]) to support a variety of external programs with specific research focuses. These joint programs have objectives consistent with the strategies of the corresponding ARO Program. Due to the unique nature of these cooperative efforts, each externally-funded effort is discussed within the chapter of the aligned scientific Division (see CHAPTERS 3-11).

II. ARO CORE (BH57) RESEARCH PROGRAM

ARO's Core Research Program is funded with Army basic research "BH57" funds and represents the primary basic research funding provided to ARO by the Army. Within this program and its ongoing BAA, research proposals are sought from educational institutions, nonprofit organizations, and commercial organizations for basic research in electronics, physics, and the chemical, computing, life, materials, mathematical, mechanical, and network sciences. The goal of this program is to utilize world-class and worldwide academic expertise to discover and exploit novel scientific discoveries, primarily at universities, to provide the current and future force with critical new or enhanced capabilities.

ARO Core Research Program activities fall under five categories, discussed in the following subsections: (a) Single Investigator awards, (b) Short Term Innovative Research efforts, (c) Young Investigator Program, (d) support for conferences, workshops, and symposia, (e) international programs, and (f) special programs. ARO's Core (BH57) Research Program represents the principal mission of ARO and is where the majority of the Army funds are used. A summary of the Core (BH57) Research Program budget is presented in Section XIII.

A. Single Investigator (SI) Program

The goal of the SI program is to pursue the most innovative, high-risk, and high-payoff ideas in basic research. Research proposals within the SI Program are received throughout the year in a continuously-open, worldwide BAA solicitation. This program focuses on basic research efforts by one or two faculty members along with supporting graduate students and/or postdoctoral researchers and is typically a three-year grant.

B. Short Term Innovative Research (STIR) Program

The objective of the STIR Program is to explore high-risk initial proof-of-concept ideas within a nine-month timeframe. Research proposals are sought from educational institutions, nonprofit organizations, or private industry. If a STIR effort's results are promising, the investigator may be encouraged to submit a proposal to be evaluated for potential longer-term funding options, such as an SI award.

C. Young Investigator Program (YIP)

The objective of the YIP is to attract outstanding young university faculty to Army-relevant research questions, to support their research, and to encourage their teaching and research careers. Outstanding YIP projects may be considered for the prestigious PECASE award (see Section IV).

D. Conferences, Workshops, and Symposia Support Program

The ARO Core Program also provides funding for organizing and facilitating scientific and technical conferences, workshops, and symposia. This program provides a method for conducting scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army and help define research needs, thrusts, opportunities, and innovation. In particular, workshops are a key mechanism ARO uses to identify new research areas with the greatest opportunities for scientific breakthroughs that will revolutionize future Army capabilities.

E. International Programs

Beginning in FY16, ARO initiated international programs with the goal of identifying academic investigators who are the forerunners in particular fields of research of which U.S. scientists do not currently hold the lead. Based on a detailed data analytics study that assessed 39 countries and their research publication output from 2009-2014, ARO identified seven scientific areas critical to the future Army, components of which are led by researchers outside of the U.S. These areas were grouped into three key geographic locations: the Atlantic, Pacific, and Americas regions.

These international programs are part of ARL and ARO's comprehensive approach to ensure that Army basic research funds are used efficiently to find the scientists best suited to drive high-risk, high-payoff Army crucial research, regardless of whether these researchers are in the U.S. or abroad. The seven ARO International Program Managers (PMs) are each aligned to an ARO Division and focus on key research areas to identify international investigators with skills and ideas in areas not led by researchers within the U.S., as well as to engage and partner those researchers with existing Army and DoD programs. These international research areas, the corresponding aligned Division, and the locations where the International PMs are stationed are listed below.

- Energy Transport and Storage (Chemical Sciences Division) - Tokyo, Japan
- Advanced Computing (Computing Sciences Division) - São Paulo, Brazil
- Synthetic Biology (Life Sciences Division) - Tokyo, Japan
- Human Dimension (Life Sciences Division) - London, United Kingdom
- Innovation in Materials (Materials Science Division) - London, United Kingdom (currently vacant)
- Network Science and Intelligent Systems (Network Sciences Division) - London, United Kingdom
- Quantum Scale Materials (Physics Division) - Tokyo, Japan

F. Special Programs

Although the programs listed earlier in this section constitute the primary use of BH57 funds, the ARO Core Research Program also supports a variety of special programs. The Research Instrumentation (RI) Program is designed to improve the capabilities of U.S. institutions of higher education to conduct research and educate scientists and engineers in areas important to national defense, and funds may be provided to purchase instrumentation in support of this research or in the development of new research capabilities. However, the majority of instrumentation support awarded through ARO is provided through the Defense University Research Instrumentation Program (see Section V). The ARO Core Research Program also co-funds awards selected through the Army's High School Apprenticeship Program (HSAP) and Undergraduate Research Apprenticeship Program (URAP), which is managed through ARO's Youth Science Activities (see Section XI).

III. MULTIDISCIPLINARY UNIVERSITY RESEARCH INITIATIVE (MURI)

As described in Section I, the MURI Program is part of the University Research Initiative (URI) and supports research teams whose research efforts intersect more than one traditional discipline. A multidisciplinary effort can accelerate research progress in areas particularly suited to this approach by cross-fertilization of ideas, can hasten the transition of basic research findings to practical applications, and can help to train students in science and/or engineering in areas of importance to DoD. In contrast with ARO Core program SI research projects, MURI projects support centers whose efforts require a large and highly collaborative multidisciplinary research effort. These are typically funded at $1.25 million per year for three years with an option for two additional years. The efforts are expected to enable more rapid research and development breakthroughs and to promote eventual transition to Army applications.

Oversight of the MURI program comes from the Basic Research Office of ASD(R&E) to the Service Research Offices (OXRs), where OXR PMs manage the MURI projects. The OXRs include ARO, the Air Force Office of Scientific Research (AFOSR), and the Office of Naval Research (ONR). OXR PMs have significant flexibility and discretion in how the individual projects are monitored and managed, while ASD(R&E) defends the program to higher levels in OSD and has responsibility for overall direction and oversight. Selection of Army research topics and the eventual awards are reviewed and approved by ASD(R&E) under a formal acquisition process.

Seven MURI projects were selected for funding and began in FY17. These projects are based on proposals submitted to the FY17 MURI topic BAA, which was released in late FY16. Each new-start project, lead investigator, and lead performing organization are listed here, immediately below the corresponding MURI topic, topic authors/PMs, and the ARO Division responsible for monitoring the project. A description of each project can be found in the corresponding Division's chapter, based on the topic's lead author.

The following 7 proposals were selected to be the FY17 new starts for the MURI Program.

- *Additive 3D Self-Assembly of Responsive Materials*; PMs: Dr. John Prater (Materials Science), and Dr. Dawanne Poree (Chemical Sciences)

  Project Selected: *Adaptive Self-Assembled Systems: Exploiting Multifunctionality for Bottom-up Large-scale Engineering*, Professor Anna Balazs, University of Pittsburgh
- *Anyons in 2D Materials and Cold Atomic Gases*; PMs: Dr. Paul Baker (Physics), Dr. Marc Ulrich (Physics), and Dr. Pani Varanasi (Materials Science)

  Project Selected: *Bottom-Up Anyons in Interacting Quantum Systems*, Professor Andrea Young, University of California - Santa Barbara
- *Information Content in Data for Multimodal Data Analysis*; PM: Dr. Liyi Dai (Computing Sciences)

  Project Selected: *Semantic Information Pursuit for Multimodal Data Analysis*, Professor Rene Vidal, Johns Hopkins University
- *Nutritional and Environmental Effects on the Gut Microbiome and Cognition*; PMs: Dr. Frederick Gregory (Life Sciences) and Dr. Robert Kokoska (Chemical Sciences)

  Project Selected: *Dissecting Microbiome-gut-brain Circuits for Microbial Modulation of Host Cognition in Response to Diet and Stress*, Professor Elaine Hsiao, University of California, Los Angeles
- *Spectral Decomposition and Control of Strongly Coupled Nonlinear Interacting Systems*; PMs: Dr. Samuel Stanton (Mechanical Sciences) and Dr. Matthew Munson (Mechanical Sciences);

  Project Selected: *From Data-Driven Operator Theoretic Schemes to Prediction, Inference and Control of Systems*, Professor Igor Mezic, University of California Santa Barbara
- *Room Temp Exciton-Polaritonics*; PMs: Dr. Michael Gerhold (Electronics) and Dr. Marc Ulrich (Physics)

  Project Selected: *Room-Temperature Two-Dimensional Polaritronics with Van der Waals Heterostructures*, Professor Hui Deng, University of Michigan
- *Cyber Deception Through Active Leverage of Adversaries' Cognition Process*; PMs: Dr. Cliff Wang (Computing Sciences) and Dr. Lisa Troyer (Life Sciences)

  Project Selected: *Realizing Cyber Inception: Towards a Science of Personalized Deception for Cyber Defense*, Professor Milind Tambe, University of Southern California

The following 8 topics were published in FY17 and constitute the ARO portion of the FY18 MURI BAA.

- *Integrated Quantum Sensing and Control for High Fidelity Qubit Operations*
  PMs: Dr. T.R. Govindan (Physics) and Dr. Samuel Stanton (Mechanical Sciences)
- *Novel solid- state materials and color centers for quantum science and engineering*
  PMs: Dr. Pani Varanasi (Materials Science), Dr. T.R. Govindan (Physics), and Dr. Paul Baker (Physics)
- *Controlling Protein Function Using Dynamic Chemical Switches to Modulate Structure*
  PMs: Dr. Stephanie McElhinny (Life Sciences) and Dr. Dawanne Poree (Chemical Sciences)
- *Consolidation of Novel Materials and Macrostructures from a Dusty Plasma*
  PMs: Dr. Michael Bakas (Materials Science), Dr. Richard Hammond (Physics), and Dr. James Parker (Chemical Sciences)
- *Embodied Learning and Control*
  PM: Dr. Samuel Stanton (Mechanical Sciences)
- *Coevolution of Neural, Cognitive, & Social Networks: Mind-Body-Community Connections*
  PMs: Dr. Edward T. Palazzolo (Network Science) and Dr. Frederick Gregory (Life Sciences)
- *Network Games*
  PMs: Dr. Purush Iyer (Network Science) and Dr. Edward Palazzolo (Network Science)
- *Modeling Interdependence among Natural Systems and Human Population Dynamics*
  Dr. Lisa Troyer (Life Sciences) and Dr. Derya Cansever (Network Science)

IV. PRESIDENTIAL EARLY CAREER AWARD FOR SCIENTISTS AND ENGINEERS (PECASE)

The PECASE program, also part of the URI program, attracts outstanding young university faculty members, supporting their research, and encouraging their teaching and research careers. PECASE awards are the highest honor bestowed by the Army to extramural scientists and engineers beginning their independent research careers. Each award averages $200K/year for five years. PECASE awards are based in part on two important criteria: (i) innovative research at the frontiers of science and technology that is relevant to the mission of the sponsoring agency, and (ii) community service demonstrated through scientific leadership, education, and outreach.

The PECASE winners for each calendar year's competition are announced by the White House. The winners of the 2014 PECASE competition were announced in FY17. Of the candidates nominated by ARO for the 2014 PECASE competition, three investigators were selected to receive PECASE awards and were announced in FY17. These awards began as "new start" projects in FY17 and are listed in this section, with the project title followed by the principal investigator (PI), performing organization, ARO PM and corresponding scientific division. Additional details for these projects can be found in the corresponding scientific division's chapter.

- *Programing Biomolecular Nanodevices For Targeted Immune Cell Recognition and Payload Delivery*
  PI: Professor Shawn Douglas, University of California - San Francisco
  ARO PM: Dr. Stephanie McElhinny, Life Sciences Division
- *Stabilization of Reactive Chemical Species and Fundamental Studies of Small-Molecule Reactivity in Metal-Organic Frameworks*
  PI: Professor Thomas Harris, Northwestern University
  ARO PM: Dr. Dawanne Poree, Chemical Sciences Division
- *Novel Quantum Phases in Heavy d- and f-electron Systems Studied Using Nonlinear Optics*
  PI: Professor David Hsieh, California Institute of Technology
  ARO PM: Dr. Marc Ulrich, Physics Division

V. DEFENSE UNIVERSITY RESEARCH INSTRUMENTATION PROGRAM (DURIP)

DURIP, also part of the URI program, supports the purchase of state-of-the-art equipment that augments current university capabilities or develops new capabilities to perform cutting-edge defense research. DURIP meets a critical need by enabling university researchers to purchase equipment costing $50K or more to conduct DoD-relevant research. In FY17, the Army awarded 56 grants at $11.1M total, with an average award of $342K.

VI. UNIVERSITY AFFILIATED RESEARCH CENTERS (UARCS)

The Army's University Affiliated Research Centers (UARCs) are strategic DoD-established research organizations at universities. The UARCs were formally established in May 1996 by ASD(R&E) in order to advance DoD long-term goals by pursuing leading-edge basic research and to maintain core competencies in specific domains unique to each UARC, for the benefit of DoD. One DoD Agency is formally designated by ASD(R&E) to be the primary sponsor for each UARC. The primary sponsor ensures DoD UARC management policies and procedures are properly implemented. Collaborations among UARCs and the educational and research resources available at the associated universities can enhance each UARC's ability to meet the long-term goals of DoD. ARO is the primary sponsor for two UARCs, with involvement in a third.

- The Army's Institute for Soldier Nanotechnologies (AISN), located at the Massachusetts Institute of Technology (MIT). The AISN is discussed further in CHAPTER 3: CHEMICAL SCIENCES DIVISION.
- The Army's Institute for Collaborative Biotechnologies (AICB), located at the University of California - Santa Barbara, with academic partners at MIT and the California Institute of Technology. The AICB is discussed further in CHAPTER 6: LIFE SCIENCES DIVISION.
- The Army's Institute for Creative Technologies (AICT), located at the University of Southern California. In contrast to the AISN and AICB, the AICT is co-managed within ARL by both ARO and the Human Research and Engineering Directorate (HRED). Funding for the AICT is managed through ARO while HRED provides technical guidance with ARO support.

VII. MINERVA RESEARCH INITIATIVE (MRI)

The Minerva Research Initiative (MRI) is a DoD-sponsored, university-based social science basic research program initiated by the Secretary of Defense and focuses on areas of strategic importance to U.S. national security policy. It seeks to increase the intellectual capital in the social sciences and improve DoD's ability to address future challenges and build bridges between DoD and the social science community. Minerva brings together universities, research institutions, and individual scholars and supports multidisciplinary and cross-institutional projects addressing specific topic areas determined by DoD.

Minerva projects are funded up to a five-year base period, with awards ranging from small, single investigator grants for 2-3 years to large multidisciplinary projects for $1-2 million per year for 5 years. The program is tri-service managed, with ARO managing 2-5 year projects dealing with causes and consequences of regime change, development of new models to pinpoint sources and effects of protest movements, relationships between natural disasters and sociopolitical instability, identification of demographic factors contributing to rise of global violent extremist organizations. ARO also provides scientific, technical, and managerial support to OSD in formulating the overall program.

The management of the OSD MRI program transitioned to the ARO Life Sciences division beginning in FY16. The titles of ARO-managed FY17 new-start Minerva projects are listed below, followed by the name of the lead PI, the performing organization, and the award duration.

- *Russian, Chinese, Militant, and Ideologically Extremist Messaging on the United States Favorability Perceptions in Central Asia*, PI: Professor Eric McGlinchey, George Mason University, FY17-FY20
- *The Youth Bulge and National Security in Africa: A Ground-Level Analysis,* PI: Professor Parfait Eloundou-Enyegue, Cornell University, FY17-FY20
- *Refugee Flows and Instability,* PI: Professor Alex Braithwaite, University of Arizona, FY17-FY120
- *Armed Conflict beyond Insurgency and Counterinsurgency: Comparative Evidence from Latin America and South Asia*, PI: Professor Paul Staniland, University of Chicago, FY17-FY20

VIII. SMALL BUSINESS INNOVATION RESEARCH (SBIR) AND SMALL BUSINESS TECHNOLOGY TRANSFER (STTR) PROGRAMS

Congress established the SBIR and STTR programs in 1982 and 1992, respectively, to provide small businesses and research institutions with opportunities to participate in government-sponsored R&D. The DoD SBIR and STTR programs are overseen and administered by the Office of Small Business Programs within the Office of the Under Secretary of Defense for Acquisition, Technology and Logistics. The Army-wide SBIR Program is managed by RDECOM, while the Army-wide STTR Program is managed by ARO. In contrast to the basic research programs managed by ARO, the SBIR and STTR programs focus primarily on feasibility studies leading to specific applications.

A. Purpose and Mission

The purpose of the SBIR and STTR programs is to (i) stimulate technological innovation, (ii) use small business to meet Federal R&D needs, (iii) foster and encourage participation by socially and economically disadvantaged small business concerns (SBCs), in technological innovation, and (iv) increase private sector commercialization of innovations derived from Federal R&D, thereby increasing competition, productivity, and economic growth. The STTR program has the additional requirement that small companies must partner with universities, federally funded research and development centers, or other non-profit research institutions to work collaboratively to develop and transition ideas from the laboratory to the marketplace.

B. Three-phase Process

The SBIR and STTR programs use a three-phase process, reflecting the high degree of technical risk involved in funding research, and developing and commercializing cutting edge technologies. The basic parameters of this three-phase process for both programs within the Army are shown in TABLE 1.

1. Phase I. Phase I of the SBIR and STTR programs involves a feasibility study that determines the scientific, technical, and commercial merit and feasibility of a concept. Each SBIR and STTR BAA contains topics seeking specific solutions to stated government needs. Phase I proposals must respond to a specific topic in the BAA, and proposals are competitively judged on the basis of scientific, technical, and commercial merit. The Phase I evaluation and award process marks the entry point to the program and cannot be bypassed.

2. Phase II. Phase II represents a major research and development effort, culminating in a well-defined deliverable prototype (*i.e.*, a technology, product, or service). The Phase II selection process is also competitive. Phase I contractors can submit Phase II proposals during one of the respective program's submissions cycles, as there are no separate Phase II BAAs. Typically 50% of Phase II proposals are selected for award. SBIR Phase II awardees may be selected to receive additional funds as an invited Subsequent Phase II, Phase II Enhancement, or via the Commercialization Readiness Program (CRP). STTR Phase II awards may also be selected to receive additional funds as an invited Subsequent Phase II.

3. Phase III. In Phase III, the small business or research institute is expected to obtain funding from the private sector and/or non-SBIR/STTR government sources to develop products, production, services, R&D, or any combination thereof into a viable product or service for sale in military or private sector markets. Commercialization is the ultimate goal of the SBIR and STTR programs.

TABLE 1

Three-phase process of the SBIR and STTR programs. Phase I is an assessment of technical merit and feasibility, Phase II is a larger R&D effort often resulting in a deliverable prototype, and Phase III is a project derived from, extending, or logically concluding prior SBIR/STTR work, generally to develop a viable product or service for military or commercial markets.

	SBIR Contract Limits	STTR Contract Limits
Phase I	• 6 months, \$100K max • 3-month option (at Government's discretion), \$50K max, to fund interim Phase II efforts	• 6 months, \$150K max • No options
Phase II	• 2 years, \$1 million max	• 2 years, \$1 million max
Subsequent Phase II	• 2 years, \$1 million max	• 2 years, \$1 million max
Phase II Enhancement	• 2 years, \$500K matching funds max	n/a
Phase III	• No time or size limit • No SBIR/STTR set-aside funds	• No time or size limit • No SBIR/STTR set-aside funds

C. ARO FY17 SBIR and STTR Topics

The following SBIR topics were published in an FY17 SBIR BAA. The lead topic author (who serves as the topic PM) and corresponding Division are listed with each topic.

- *Biologically-Derived Targeted Antifungals for Textile Applications*; Dr. Stephanie McElhinny, Life Sciences
- *CMOS Compatible Deposition of Multi-Ferroic Films for Tunable Microwave Applications*; Dr. James Harvey, Electronics
- *Lithium Ion Battery Electrodes Manufacturing to Improve Power and Energy Performance*; Dr. Robert Mantz, Chemical Sciences
- *Low Cost, Compact, and High Power Terahertz Emitter Arrays with 1550-nm Telecommunications Laser Drivers*; Dr. Joe Qiu, Electronics
- *Cryogenic Optical Connector for Focal Plane Array Read-out*; Dr. Michael Gerhold, Electronics
- *Lead Acid Battery Monitoring, Diagnostics, and Prognostics*; Dr. Robert Mantz, Chemical Sciences

The following STTR topics were published in an FY17 STTR BAA. The lead topic author and corresponding Division are listed following each topic title.

- *Mid-Infrared Chip-scale Trace Gas Sensors*; Dr. Michael Gerhold, Electronics
- *Mid-wave Infrared Laser Beam Steering*; Dr. Michael Gerhold, Electronics
- *High Dynamic Range Heterodyne Terahertz Imager*; Dr. Joe Qiu, Electronics

- *3D Tomographic Scanning Microwave Microscopy with Nanometer Resolution*; Dr. Joe Qiu, Electronics
- *Mechanochemical Sensing and Self Healing Solution to Detecting Damage in Composite Structures*; Dr. David Stepp, Engineering Sciences
- *Scientific Data Management via Fast Dynamic Summarization*; Dr. Joseph Myers, Mathematical Sciences
- *Synthetic Biology Toolkit for Bioconversion of Food Waste*; Dr. Aura Gimm, Physical Sciences
- *High Performance Armor via Additive Advanced Ceramics*; Dr. Stephen Lee, Chemical Sciences
- *Scalable Manufacturing of Functional Yarns for Textile-based Energy Storage*; Dr. Robert Mantz, Chemical Sciences
- *Biosensor for Detection of Synthetic Cannabinoids*; Dr. Stephanie McElhinny, Life Sciences
- *Sealed Container Content Identification*; Dr. Dawanne Poree, Chemical Sciences
- *Method for Locally Measuring Strength of a Polymer-Inorganic Interface During Cure and Aging*; Dr. Dawanne Poree, Chemical Sciences

D. ARO FY17 SBIR and STTR Phase II Contract Awards

The following SBIR and CBD SBIR topics were selected for Phase II contracts in FY17. The lead topic author/PM and corresponding Division are listed following each topic title.

- *High Quality Factor, Thin-Film, Electrically Tunable Varactors and Filters*; Dr. James Harvey, Electronics
- *HGCDTE Material Improvements for High Operating Temperatures*; Dr. Michael Gerhold, Electronics
- *Wireless Networking Using Multiple Antenna Interference Alignment*; Dr. Robert Ulman, Network Sciences
- *Enhanced Analysis for Pulsed Voltammetry Evaluation Tool / System for Improved Power Systems*; Dr. Robert Mantz, Chemical Sciences
- *Low-Loss Commercial Deposition Technology for Thick Ferrites and Ferrite/Insulator Films on Printed Circuit Boards*; Dr. James Harvey, Electronics

The following STTR and CBD STTR topics were selected for Phase II contracts in FY17. The lead topic author/PM and corresponding Division are listed following each topic title.

- *Lithium Ion / Super Capacitor Hybrid System*; Dr. Robert Mantz, Chemical Sciences
- *Ultra-Coherent Semiconductor Laser Technology*; Dr. Michael Gerhold, Electronics
- *Powerful Source of Collimated Coherent Infrared Radiation with Pulse Duration Fewer than Ten Cycles*; Dr. James Harvey, Electronics
- *High-Performance Magnesium Alloys and Composites by Efficient Vapor Phase Processing*; Dr. David Stepp, Engineering Sciences
- *Circadian Rhythm Monitoring and Regulation Device*; Dr. Virginia Pasour, Mathematical Sciences
- *Vacuum Integrated System for Ion Trapping*; Dr. TR Govindan, Physics
- *Parallel Two-Electron Reduced Density Matrix Based Electronic Structure Software for Highly Correlated Molecules and Materials*; Dr. Jim Parker, Chemical Sciences
- *Compressive Sensing Flash IR 3D Imager*; Dr. Liyi Dai, Computing Sciences
- *EMS Monitor & Broadcast Training Capacity Enhancement*; Dr. Robert Ulman, Network Sciences
- *Development of a Forensic Swab for High Efficiency Capture and Release of DNA*; Dr. Stephanie McElhinny, Life Sciences
- *Automated Deployable Robust Training System*; Dr. Micheline Strand, Life Sciences
- *Hybrid Battery/Supercapacitor Energy Storage Device*; Dr. Robert Mantz, Chemical Sciences
- *Parallel Adaptive Simulation of Multiphase Ballistic Flows*; Dr. Joseph Myers, Mathematical Sciences

- *Freeze Casting of Tubular Sulfur Tolerant Materials for Solid Oxide Fuel Cells*; Dr. Robert Mantz, Chemical Sciences
- *Acoustically/Vibrationally Enhanced High Frequency Electromagnetic Detector for Buried Landmines*; Dr. James Harvey, Electronics
- *Novel OSINT Platform for Enhanced OSINT Collection*; Dr. Edward Palazzolo, Network Sciences
- *QADE: Quantification, Analysis, Defense and Evaluation System for Resilient and Secure Wireless Communication Operations*; Dr. Cliff Wang, Computing Sciences
- *Field Drug Identification Kit*; Dr. Dawanne Poree, Chemical Sciences

E. ARO FY17 SBIR and CBD SBIR Subsequent Phase II Contract Awards

The following SBIR and CBD SBIR topics were selected for Su Phase II contracts in FY17. The lead topic author/PM and corresponding Division are listed following each topic title.

- *Portable JP8-Fueled Solid Acid Fuel Cell Power Unit*; Dr. Robert Mantz, Chemical Sciences
- *Social and Psychological Meaning in Social Media*; Dr. Leonard Wilkins, Mathematical Sciences
- *Nanostructured Electrode Materials for Enhanced Biological Charge Transfer*; Dr. Stephanie McElhinny, Life Sciences
- *Fabrication of High-Strength, Lightweight Metals for Armor and Structural Applications*; Dr. David Stepp, Engineering Sciences
- *Quantum Noise Controlled Laser for Integrated Photonics*; Dr. Michael Gerhold, Electronics
- *Long-Term Reliable, High-Power Midwave-Infrared Quantum Cascade Lasers*; Dr. Michael Gerhold, Electronics
- *Doping and Compensation Control in AlGaN for High Power Devices*; Dr. Chakrapani Varanasi, Materials Science
- *Direct Ethanol Fuel Cell*; Dr. Robert Mantz, Chemical Sciences
- *Global Spatiotemporal Disease Surveillance System*; Dr. Bob Kokoska, Life Sciences
- *Producing Novel Biosynthetic Therapeutics from Extreme Microbiomes*; Dr. Bob Kokoska, Life Sciences

F. ARO FY17 STTR and CBD STTR Subsequent Phase II Contract Awards

The following STTR topics were selected for Subsequent Phase II contracts in FY17. The lead topic author/PM and corresponding Division are listed following each topic title.

- *Nondestructive Concrete Characterization System*; Dr. Dawanne Poree, Chemical Sciences
- *Liquid Crystal-based Sensors for Detection of Airborne Toxic Chemicals for Integration with Unmanned Robotic Systems*; Dr. Dawanne Poree, Chemical Sciences
- *Development of comprehensive biothreat identifier - Zeteo Threat Agent Detection System (zTADS)*; Dr. Dawanne Poree, Chemical Sciences

G. ARO FY17 SBIR and CBD SBIR Phase III Contract Awards

The following SBIR and CBD SBIR topics were awarded a Phase III contract in FY16 and FY17. The lead topic author/PM and corresponding Division are listed following each topic title. Phase III revenues can be obtained from Government or private customers, but cannot be SBIR/STTR funds.

- *Advancement of Capabilities, Products, and Sensors in Chem/Bio Detection, Quantification, and Mitigation IDIQ*; Dr. Stephen Lee, Chemical Sciences
- *ID/IQ for USASOC Engineering Analysis and Support*; Dr. Stephen Lee, Chemical Sciences
- *Equipment Sets for Mitigating Advanced Threats*; Dr. Stephen Lee, Chemical Sciences

H. ARO FY17 STTR Phase III Contract Awards

The following STTR topic was awarded a Phase III contract in FY17. The lead topic author/PM and corresponding Division are listed following the topic title. Phase III revenues can be obtained from Government or private customers, but cannot be SBIR/STTR funds.

- *On Demand Energy Activated Liquid Decontaminants and Cleaning Solutions*; Dr. Dawanne Poree, Chemical Sciences

I. Contract Evaluation and Funding

The Army receives Phase I and Phase II proposals in response to SBIR, STTR, CBD-SBIR/STTR and OSD-SBIR/STTR topics that are published during solicitation periods throughout each fiscal year. Proposals are evaluated against published evaluation criteria and selected for contract award. Contract awards are made pending completion of successful negotiations with the small businesses and availability of funds.

IX. HISTORICALLY BLACK COLLEGES AND UNIVERSITIES AND MINORITY-SERVING INSTITUTIONS (HBCU/MSI) PROGRAMS

Programs for HBCU/MSIs are a significant part of the ARO portfolio. Awards in FY17 totaled $25.1 million. These programs are discussed in the following subsections.

A. ARO (Core) HBCU/MSI Program

Academic institutions classified as HBCU/MSIs may submit proposals to the ARO Core BAA, as for any other institution, and are evaluated and selected according to the same evaluation criteria and process established for all proposal submissions to the Core BAA. In FY17, ARO supported 89 agreements with HBCU/MSI institutions receiving over $9.9 million in FY17 funding, including 18 new starts listed below.

The new-start HBCU/MSI research grants are listed below, with the project title followed by the PI, performing organization, ARO PM, and corresponding scientific division.

- *Ballistic Holography under Realistic Spray Conditions,* Professor Derek Dunn-Rankin, University of California – Irvine; Dr. Ralph Anthenien, Mechanical Sciences Division
- *Nanomechanical Systems with Normalized and Coupled Acoustic and Electromagnetic Modes in Piezoelectric Structures*, Professor Michael Stroscio, University of Illinois - Chicago; Dr. James Harvey, Electronics Division
- *Multi-Dimensional and Dissipative Dynamical Systems: Maximum Entropy as a Principle for Modeling Dynamics and Emergent Phenomena in Complex Systems*, Professor Steve Presse, Arizona State University; Dr. Samuel Stanton, Mechanical Sciences Division
- *Alloys of Transition Metal Trichalcogenides for New-class of Two-dimensional Materials with Infrared Bandgaps*, Professor Sefaattin Tongay, Arizona State University; Dr. Chakrapani Varanasi, Materials Science Division
- *Algorithms for Visualization and Simulation of Optimal Navigation*, Professor Marcelo Kallmann, University of California – Merced; Dr. J. Michael Coyle, Computing Sciences Division
- *Ninth International Workshop on Network Science for Communication Networks (NetSciCom)*, Professor Arunabha Sen, Arizona State University; Dr. Alfredo Garcia, Network Sciences Division
- *A Deep Learning Framework for Network Dynamics Prediction*, Professor Justin Zhan, University of Nevada - Las Vegas; Dr. Purush Iyer, Network Sciences Division
- *Mathematical Sciences - Field Control through Submanifold Active Manipulation in CED*, Professor Daniel Onofrei, University of Houston; Dr. Joseph Myers, Mathematical Sciences Division

- *Workshop on Dynamics, Control and Numerics of Fractional Partial Differential Equations,* Professor Mahamadi Warma; University of Puerto Rico at Rio Piedras; Dr. Joseph Myers, Mathematical Sciences Division
- *Non-equilibrium Statistical Mechanics and Curvature*, Professor Tryphon Georgiou, University of California - Irvine; Dr. Joseph Myers, Mathematical Sciences Division
- *Predicting Tissue Dynamics based on Stochastic Variations in Cell Stiffness and Spatial Clustering within the Tissue Environment*, Professor Parag Katira, San Diego State University; Dr. Virginia Pasour, Mathematical Sciences Division
- *Transient Behavior of Organisms Responding to Sudden Cues*, Professor Daisuke Takagi, University of Hawaii - Honolulu; Dr. Virginia Pasour, Mathematical Sciences Division
- *Multi-layer Resilient Active Cyber Defense - Metrics, Synthesis, Evaluation and Verification*, Professor Ehab Al-Shaer, University of North Carolina - Charlotte; Dr. Cliff Wang, Computing Sciences Division
- *MTD Dynamics: A Quantative Framework for Modeling and Orchestrating Moving-Target Defense*, Professor Shouhuai Xu, University of Texas at San Antonio; Dr. Cliff Wang, Computing Sciences Division
- *Workshop on HoneyThings: Automated and Dynamic Cyber Deception,* Professor Jinpeng Wei, University of North Carolina - Charlotte; Dr. Cliff Wang, Computing Sciences Division
- Microbial Consortia and Biofilms Workshop, Professor Michelle O'Malley, University of California – Santa Barbara; Dr. Robert Kokoska, Life Sciences Division
- Probing the Surfaces of Atmospheric Organic Particles and the Implications for Climate Change, Air Quality, Visibility and Bioavailability, Professor Barbara Finlayson-Pitts, University of California - Irvine; Dr. James Parker, Chemical Sciences Division
- *Quantitative and Mechanistic Analyses of Bond Selective Chemistry via Non-Thermal Excitation of Metal Nanostructures,* Professor Phillip Christopher, University of California - Riverside; Dr. Robert Mantz, Chemical Sciences Division

As for all institutions funded through the ARO Core Program, HBCU/MSI institutions selected for funding were afforded the opportunity to submit add-on proposals to fund high school or undergraduate student research apprenticeships through HSAP/URAP. A total of 23 HBCU/MSIs were funded under HSAP/URAP in FY17, totaling approximately $167K, (50/50 mix of PM and Army Education Outreach Program funding). Additional information regarding HSAP/URAP can be found in Section XI: *Youth Science Activities*.

B. Partnered Research Initiative (PRI)

The PRI Program was established as the next phase of what was previously known as the Partnership in Research Transition (PIRT) Program, which ended in FY16. The focus of the PRI Program is to advance innovative basic research leading to potential technology development in areas of strategic importance to the Army by bringing competitively selected HBCU/MSI research teams into existing ARL Collaborative Research Alliances (CRAs) and Collaborative Technology Alliances (CTAs). The CTAs and CRAs are large collaborative centers focused on developing and transitioning research in Army critical areas. In FY17, ARL's PRI Program for HBCUs/MSIs selected four projects totaling $1.35 million to join the CTA/CRA consortia from 142 candidate whitepapers submitted. The New Mexico Institute of Mining and Technology joined the Multiscale Modeling of Electronic Materials CRA, City College of New York joined the Cognition and Neuroergonomics CTA, University of Texas at El Paso joined the Cyber Security CRA, and North Carolina Agricultural and Technical State University joined the Materials in Extreme Dynamic Environments CRA. The projects listed below will be funded for up to four years and will be performed in collaboration with ARL and CTA/CRA member institutions to maximize the impact of the research and enhance HBCU/MSI research capabilities.

- PRI Title: *Defeating the Dark Triad in Cyber-security Using Game Theory*
  Integrated into Cyber Security CRA
  CTA/CRA Collaborating Institution: University of Texas at El Paso
  PI: Professor Christopher Kiekintveld
  Cooperative Agreement Manager (CAM): Dr. Edward Colbert

- PRI Title: *Material Design Under Uncertainty*
  Integrated into Multiscale Modeling of Electronic Materials (MSME) CRA
  CTA/CRA Collaborating Institution: New Mexico Institute of Mining and Technology (NMT)
  PI: Dr. Yanyan He
  CAM: Dr. Meredith Reed
- PRI Title: *Tailoring Mg-alloy Systems through Composition /Microstructure/Severe Plastic Deformation for Army Extreme Dynamic Environment Applications*
  Integrated into Materials in Extreme Dynamic Environments (MEDE) CRA
  CTA/CRA Collaborating Institution: North Carolina A&T State University
  PI: Dr. Jagannathan Sankar
  CAM: Dr. John Beatty
- PRI Title: *Reliability of Neural Activity as an Assay of Cognitive State*
  Integrated into Cognition and Neuroergonmics (CaN) CTA
  CTA/CRA Collaborating Institution: City College of New York (CCNY)
  PI: Dr. Jacek Dmochowski
  CAM: Dr. Jon Touryan

C. DoD Research and Educational Program (REP) for HBCU/MSIs

ARO has administered programs on behalf of ASD(R&E) since 1992. REP aims to enhance research capabilities of HBCUs and MSIs and to strengthen their education programs in science, technology, engineering, and mathematics (STEM) disciplines that are relevant to the defense mission.

Under this program, qualifying institutions were able to submit proposals to compete for basic research grants. In FY17, BAA W911NF-16-R-0024 was issued for the DoD REP for HBCUs/MSIs, with 138 proposals identified as eligible under the solicitation. In FY17, 47 grants totaling $20.7 million were made, 18 to HBCUs, 26 to MSIs, 2 to TCUs and 1 to a Predominately Black Institution (PBI) under the DoD REP solicitation.

D. Other HBCU/MSI Activities

On 29 June 2017, ARO hosted a Department of Defense Research Workshop for HBCU/MIs from across the country, in partnership with the Basic Sciences Office of the Assistant Secretary of Defense (Research and Engineering). The event, attended by over 190 registered participants representing at least 66 HBCU/MSIs, provided a comprehensive overview of DoD research funding and partnering opportunities and offered basic training on how to do business with DoD, with focus on the proposal submission, grants, cooperative agreements and contracts. Additionally, the event featured breakout sessions for attendees to learn about specific DoD research needs through direct interaction with program managers from the Army, Navy Air Force and DARPA, to initiate dialogue in areas of shared scientific interest. The broad purpose of the event was to expand and diversify the defense research base by increasing HBCU/MSI participation in defense research.

X. NATIONAL DEFENSE SCIENCE AND ENGINEERING GRADUATE (NDSEG) FELLOWSHIP PROGRAM

The NDSEG Fellowship Program is a tri-service program administered by the Air Force Office of Scientific Research (AFOSR), designed to increase the number of US citizens trained in disciplines of science and engineering important to defense goals. ARO supports the NDSEG Fellowship Program along with the Office of Naval Research (ONR) and AFOSR. NDSEG is a highly competitive fellowship awarded to U.S. citizens who have demonstrated a special aptitude for advanced training in science and engineering, and who intend to pursue a doctoral degree in one of fifteen scientific disciplines of interest to the military. NDSEG Fellowships have historically lasted for three years, but in FY17 were extended to 4 years (just for that year group). Fellows are provided full tuition and fees at any accredited university of choice, a monthly stipend very competitive with other top-tier fellowships ($3,200/month), up to $1,500/year in medical insurance ($1,200 for subsequent year groups), and $10,000 to support travel during the duration of the fellowship ($5,000 for subsequent year groups).

With the funds made available to the Army to support candidates in FY17, ARO selected 65 NDSEG Fellows from 13 categories relevant to Army fundamental research priorities. These awardees began their fellowships in the fall of 2017. Each of ARO's divisions reviewed the applications assigned to NDSEG topic categories within their particular areas of expertise, and selected fellows whose doctoral research topics most closely align with the Army's missions and research needs. The number of Fellows chosen from each discipline was based roughly on the percentage of applicants who submitted topics in that category. The number of fellows chosen from each scientific discipline for the FY17 NDSEG program is shown in TABLE 2.

TABLE 2

FY17 NDSEG fellows by discipline. The table displays the number of NDSEG Fellows chosen in FY17, according to topic categories relevant to the designated Army research priorities.

Scientific Discipline	NDSEG Fellows Selected in FY17
Aeronautical and Astronautical Engineering	4
Biosciences	10
Chemical Engineering	5
Chemistry	6
Civil Engineering	3
Cognitive, Neural, and Behavioral Sciences	5
Computer and Computational Sciences	5
Electrical Engineering	5
Geosciences	3
Materials Science and Engineering	6
Mathematics	3
Mechanical Engineering	5
Physics	5
TOTAL	**65**

XI. YOUTH SCIENCE ACTIVITIES

All the programs managed by the Army Educational Outreach Program (AEOP) STEM Outreach Office at RDECOM Headquarters share one purpose: to increase the number of future adults with careers in science, technology, engineering, and mathematics. These programs accomplish this through a variety of mechanisms, including: providing a work/study laboratory experience, sponsoring hands-on science workshops during the summer, showcasing talented young high school scientists at symposia, and supporting student science fairs nationwide. Of these many programs, ARO continued to administer the High School and Undergraduate Research Apprenticeship Programs in FY17

During the summer of FY17, 113 students served as interns and worked in university laboratories with mentors though the High School Apprenticeship Program (HSAP) and the Undergraduate Research Apprentice Program

(URAP). This was a slight decrease from the number of participants in FY16. These programs are described further in the following subsections.

A. Undergraduate Research Apprenticeship Program (URAP)

URAP funds the STEM apprenticeship of promising undergraduates to work in university-structured research environments under the direction of ARO-sponsored PIs serving as mentors. In FY17 URAP awards provided 59 students with research experiences at 39 different universities within 23 different states. Twenty-three of the universities were HBCU/MSIs. ARO invested approximately $236K in the FY17 URAP effort, a mix of ARO core funding and AEOP matching funds.

B. High School Apprenticeship Program (HSAP)

HSAP funds the STEM apprenticeship of promising high school juniors and seniors to work in university-structured research environments under the direction of ARO-sponsored PIs serving as mentors. In FY17, HSAP awards provided 54 students with research experiences at 36 different universities within 22 different states. Twenty of the universities were HBCU/MSIs. ARO invested approximately $221K in the FY17 HSAP effort, including ARO core funding and AEOP matching funds.

C. Thurgood Marshall College Fund Pilot Initiative

The Vivian Burey Marshall Academy (VBMA), named in honor of Justice Thurgood Marshall's first wife, is a two-tiered, pilot initiative grant awarded to the Thurgood Marshall College Fund in late FY16. This is a four-year research grant award up to $5.7 million funded by ASA (ALT) through ARL’s Broad Agency Announcement and consistent with the goals of the AEOP. The pilot initiative will develop in young students, grades 6-10, STEM literacy and the basic underlying skills necessary for STEM management.

The pilot effort will be evaluated throughout the 4-year implementation to assess impact and feasibility of program adoption. ASA (ALT) has requested Army science and technology (S&T) organizations support VBMA sites for the initial year: RDECOM with Baltimore, MD, and ERDC with Vicksburg, MS.

D. Local Outreach

The Youth Sciences division of ARO participated in the following local outreach efforts in FY17.

- North Carolina Science and Engineering Fair: ARO PMs volunteered to judge posters for a special category that presents awards to high school juniors and seniors based upon the overall quality and Army relevance of their projects.
- JSHS National Symposium: scientists from ARO and sponsored PIs attended and judged student posters as well as oral presentations of students that have previously won regional competitions. Winners are awarded various scholarships ranging from $4,000 to $12,000.
- Site visits to local and out of state universities that host HSAP/URAP participants: the HSAP/URAP Program Coordinator visited ten (10) host sites in North Carolina, Texas and New York to measure program efficacy. An ARO PM accompanied the Program Coordinator on three of the visits.
- Innovation STEM Expo: ARO joined US2020 RTP, a nonprofit organization that facilitates Science, Technology, Engineering and Mathematics outreach and mentoring opportunities for underrepresented minorities, during their “Innovation STEM” expo. ARO PMs in the fields of chemistry, physics, mathematics, environmental, social and life sciences volunteered as speed mentors to an estimated 400 students ranging from grades 5 to 12 at the Frontier building in Research Triangle Park, North Carolina.
- ARO STEM Professionals Speed Mentoring Event: over 20 ARO staff members participated in a speed mentoring event with students in a one-on-one, timed rotation to share their journey from STEM education to their present career. During the speed mentoring sessions students were able to share their interests and specific questions of the mentors.

XII. SCIENTIFIC SERVICES PROGRAM (SSP)

ARO established the SSP in 1957. This program provides a rapid means for the Army, DoD, OSD, and other federal government agencies to acquire the scientific and technical analysis services of scientists, engineers, and analysts from small and large businesses, colleges and universities, academicians working outside their institutions, and self-employed persons not affiliated with a business or university. Annual assistance is provided through the procurement of short-term, engineering and scientific technical services in response to user-agency requests and funding. Through the SSP, these individuals provide government sponsors with scientific and technical results and solutions to problems related to R&D by conducting well-defined studies, analyses, evaluations, interpretations, and assessments in any S&T area of interest to the government.

SSP services are administered and managed for ARO through the Battelle Eastern Science and Technology (BEST) Center located in Aberdeen, Maryland on behalf of Battelle Memorial Institute (BMI), headquartered in Columbus, Ohio. Battelle's responsibilities include the selection of qualified individuals, universities, businesses, and/or faculty to perform all tasks requested by ARO, and for the financial, contractual, security, administration, and technical performance of all work conducted under the program.

SSP awards tasks in a wide variety of technical areas, including mechanical engineering, computer sciences, life sciences, chemistry, material sciences, and military personnel recruitment/retention. In FY17, 21 new SSP tasks were awarded with 76 modifications to the scope and/or funding of ongoing tasks. A summary of the agencies served under this program and the corresponding number of FY17 new SSP tasks is provided in TABLE 3.

TABLE 3

FY17 new SSP tasks and sponsoring agencies. In FY17, 21 new SSP tasks were awarded in addition to 106 modifications of the scope and/or funding of ongoing tasks on two SSP contracts.

Sponsoring Organization	SSP Tasks
Army Research, Development and Engineering Command (RDECOM)	
Army Research Laboratory (ARL)	2
Tank and Automotive RDEC (TARDEC)	2
Natick Soldier RDEC (NSRDEC)	2
TOTAL: RDECOM	**6**
Other U.S. Army	
U.S. Military Academy (USMA)	1
Headquarters Department of Army (HQDA)	4
U.S. Army Corps of Engineers (USACE)	2
U.S. Army Training & Doctrine Command (TRADOC)	2
U.S. Army Medical Command (MEDCOM)	2
TOTAL: Other U.S. Army	**11**
Other DoD	
U.S. Marine Corps (USMC)	2
U.S. Navy	2
TOTAL: Other DoD	**4**
TOTAL FY17 SSP Tasks	**21**

XIII. SUMMARY OF PROGRAM FUNDING AND ACTIONS

A. FY17 Research Proposal Actions

ARO PMs receive white papers throughout the year and discuss these topic ideas with the potential investigator to identify any ways the proposed research could better align with program vision and Army needs. PMs then encourage a subset of the white papers to be submitted as full proposals; however, any eligible investigator can submit a full proposal, regardless of PM recommendations. It is rare for a potential investigator to submit a full proposal without first submitting a white paper. Approximately one-third of the white papers received by ARO PMs from academic institutions are ultimately submitted as formal, full proposals. The actions for FY17 extramural basic research white papers and full proposal submissions are summarized in TABLE 4.

TABLE 4

FY17 ARO Research Proposal Actions. The status of white papers and research proposals received by ARO within FY17 (*i.e.*, 1 Oct 2016 through 30 Sep 2017) is listed for each scientific division, based on proposal actions reported through 3 May 2018. The table reports actions for extramural proposals in the basic research categories: SI, STIR, YIP, HBCU/MSI, MRI, MURI, and DURIP. White papers are defined as potential research concepts submitted to an ARO Program Manager for discussion and potential submission as a full proposal, in line with the process outlined in the ARO BAA.

	White Papers	Full Proposals				
	Received	Received	Accepted	Declined	Pending	Withdrawn
Chemical Sciences	264	129	37	51	41	0
Computing Sciences	135	79	22	33	22	2
Electronics	104	76	29	23	24	0
Life Sciences	534	93	38	29	26	0
Materials Science	409	105	40	44	20	1
Mathematical Sciences	116	79	23	17	38	1
Mechanical Sciences	140	92	31	49	12	0
Network Sciences	106	58	23	17	18	0
Physics	110	80	30	37	13	0
TOTAL	**1918**	**791**	**273**	**300**	**214**	**4**

B. Summary of ARO Core Program Budget

The ARO FY17 Core (BH57) Research Program budget is shown in TABLE 5, below.

TABLE 5

ARO Core (BH57) Program funding. The ARO Core Program FY17 Budget is listed according to each scientific discipline (Division) or special program. The FY17 Allotment totals shown here are the funds ARO had received and allotted within FY17, regardless of the year of appropriation, based on the 31 Jan 2018 transactions report from the General Fund Enterprise Business System (GFEBS) and the corresponding ARO Status of Funds Report.

ARO Core (BH57) Program Type	Division or Program Title	FY17 Allotment
Scientific Disciplines[1]	Chemical Sciences	$10,538,458
	Computing Sciences	$6,554,260
	Electronics	$7,420,026
	Life Sciences	$9,145,849
	Materials Science	$9,978,846
	Mathematical Sciences	$7,373,572
	Mechanical Sciences	$7,957,396
	Network Sciences	$8,153,004
	Physics	$9,114,111
	SUBTOTAL: Core Program Funding by Scientific Discipline	**$76,235,522**
Special Programs	Senior Scientist Research Programs	$376,486
	National Research Council (NRC) Associates Program	$211,378
	International Offices[2]	$1,768,227
	Youth Sciences Program: HSAP/URAP[3]	$193,732
	ARL General and Administrative Support	$3,155,760
	In-House Operations	$9,646,627
	SUBTOTAL: Core Program Funding to Special Programs	**$15,158,478**
TOTAL	**ARO Core (BH57) Program**	**$91,394,000**

[1] Scientific divisions also received and executed funds through the Army's Congressional Basic Research Initiatives (T14 funds; not shown here; refer to TABLE 6)

[2] Includes funds for research grants monitored through ARO International PMs (refer to Section II-E)

[3] The HSAP/URAP component of the Youth Sciences Program is funded in part through BH57 funds within each division and from the Youth Sciences Program, resulting in a total FY17 funds of $387K used to support HSAP/URAP projects

C. Summary of Other Programs Managed or Co-managed by ARO

The FY17 allotments and funding sources for other ARO managed or co-managed programs (*i.e*, not part of the ARO Core Program), are shown in TABLES 6-8.

TABLE 6

FY17 allotments for other Army-funded programs. These programs, combined with the ARO Core (BH57) Program elements shown in TABLE 5, represent all of the Army funds managed through ARO. The FY17 allotments include funds ARO received and allotted within FY17, regardless of the year of appropriation. Data source: ARO 31 Jan 2018 Status of Funds Report (for FY17 funds received in FY17) and 30 Sep 2017 Status of Funds Report (for FY16 funds received in or reallocated for FY17).

Other Army-funded Program	FY17 Allotment
Multidisciplinary University Research Initiative	$45,967,175
Presidential Early Career Award for Scientists and Engineers	$1,800,000
Defense University Research Instrumentation Program	$11,133,130
University Research Initiative Support	$4,646,695
Minerva Program (Project V72)[1]	$2,959,000
HBCU/MSI – PIRT Centers (Project H04)[2]	$3,215,000
Army Institute for Collaborative Biotechnologies (AICB; Project H05)	$6,341,000
Army Institute for Soldier Nanotechnologies (AISN; Project J12)	$5,947,000
Army Institute for Creative Technologies (AICT; Project J08)	$5,948,000
Board of Army Science and Technology (BAST; Project C18)	$805,646
Small Business Innovation Research (SBIR; Project M40)[1,3]	$11,534,694
Small Business Technology Transfer (STTR; Project 861)[1,4]	$12,443,658
SBIR/STTR Services / Contract Support (Project 720)[5]	$1,060,293
U.S. Army Medical Research and Materiel Command (MRMC)	$2,905,149
RDECOM Research, Development and Engineering Centers[6]	$3,349,294
Basic Research Initiatives – Congressional (T14)	$13,100,000
TOTAL: Other Army-funded Programs	**$133,155,734**

[1] Does not show additional funds provided by OSD (see TABLE 8)
[2] Includes $1,786,000 of FY16 funds received in or reallocated for FY17
[3] Includes $4,562,976 of FY16 funds received in or reallocated for FY17
[4] Includes $2,533,536 of FY16 funds received in or reallocated for FY17
[5] Includes $365,111 of FY16 funds received in or reallocated for FY17
[6] Includes $611,962 of FY16 funds received in or reallocated for FY17

TABLE 7

FY17 allotment for externally-funded programs. FY17 funds received from sources other than Army or OSD are indicated below. The Other Agencies category includes funds from a range of sources, such as the DoD Washington Headquarters Service (DODWHS) and the Defense Threat Reduction Agency (DTRA). Data source: 30 Sep 2017 (for FY16 funds received in or reallocated for FY17) and 31 Jan 2018 Status of Funds Reports.

External Program	FY17 Allotment
Scientific Services Program (SSP)[1]	$2,973,216
Air Force Research Laboratory (AFRL)	$5,531,646
Defense Advanced Research Projects Agency (DARPA)[2]	$174,257,798
Other Agencies (*e.g.*, DODWHS, DTRA)[3]	$170,967,244
TOTAL: External Programs	**$353,729,904**

[1] Includes $212,978 of FY16 funds received in or reallocated for FY17
[2] Includes $20,460,660 of FY16 funds received in or reallocated for FY17
[3] Includes $18,520,284 of FY16 funds received in or reallocated for FY17

TABLE 8

OSD direct-funded programs. These funds were allocated directly from OSD to the indicated program. Data source: 31 Jan 2018 Status of Funds Report.

OSD Direct-funded Programs	FY17 Allotment
SBIR/STTR (Project BP0)[1,2]	$ 1,572,574
Minerva[3]	$8,870,873
HBCU/MSI Research and Educational Program (REP)[4]	$22,556,000
TOTAL: OSD Direct Funding	**$32,999,447**

[1] Does not include additional Army funds provided for SBIR/STTR (see TABLE 6).
[2] This allotment was FY16 funds received in or reallocated for FY17
[3] Includes $6,575,648 of FY16 funds received in or reallocated for FY17
[4] This amount does not include the additional Army Core Program funds provided for the HBCU/MSI Program (see TABLE 5).

D. Grand Total FY17 Allotment for ARO Managed or Co-managed Programs

TABLE 9

Summary of FY17 allotment for all ARO managed or co-managed programs. This table lists the subtotals from TABLES 6-9 and the grand total FY17 allotment for all ARO managed or co-managed programs. The FY17 allotments include funds ARO received and allotted within that FY, regardless of the year of appropriation (e.g., FY17 allotment includes any FY16 funds received during or allocated for FY17). Refer to TABLES 6-9 for data source information.

Program Category	FY17 Allotment
Core (BH57) Programs	$91,394,000
Other Army-funded Programs	$133,155,734
External Program Funds	$353,729,904
OSD Direct-funded Programs	$32,999,447
GRAND TOTAL: (all sources)	**$611,279,085**

CHAPTER 3: CHEMICAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2017* is to provide an annual historical record summarizing the programs and basic research supported by ARO in FY17. ARO's mission is to support creative basic research resulting in new science that enables new materials, devices, processes, and capabilities for the current and future Soldier. This chapter provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions enabled by the ARO Chemical Sciences Division in FY17.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Chemical Sciences Division supports research to identify and control the fundamental properties, principles, and processes governing molecules and their interactions in materials and chemical systems that will ultimately enable critical new Army capabilities. More specifically, the Division promotes basic research to uncover the relationships between molecular architecture and material properties, to understand the fundamental processes of electrochemical reactions, to develop methods for accurately predicting the pathways, intermediates, and energy transfer of reactions, and to discover and characterize the many chemical processes that occur at surfaces and interfaces. The results of these efforts will stimulate future studies and help keep the U.S. at the forefront of chemical sciences research. In addition, these efforts are expected to lead to new approaches for synthesizing and analyzing molecules and materials that will open the door to future studies that are not feasible with current knowledge.

2. Potential Applications. Research managed by the Chemical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, results from the Chemical Sciences Program may lead to materials with new or enhanced properties to protect the Soldier from ballistic, chemical, and biological threats. The development of new computational methods may allow the structure and properties of notional (*i.e.*, theoretical) molecules to be calculated before they are created, providing a significant cost savings to the Army. This research may ultimately improve Soldier mobility and effectiveness through the development of light-weight and small power sources, renewable fuels, and new energetic materials with improved methods for ignition, deflagration, detonation, and control thereof.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Chemical Sciences Division coordinates and leverages research within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), and the Air Force Office of Scientific Research (AFOSR). The Division coordinates with other ARO Divisions to co-fund research, identify multidisciplinary research topics, and to evaluate the merit of research concepts. For example, interactions with the ARO Life Sciences Division include developing research programs to investigate materials for use in chemical and biological defense and to understand how biological systems can interface with or expand the capabilities of abiotic systems. The Chemical Sciences Division also coordinates its research portfolio with the Materials Science Division to pursue the design and characterization of novel materials through new synthesis and processing methods, the evaluation of bulk mechanical properties, and molecular-level studies of materials and material properties. The Division also complements research in the Physics and Electronics Divisions to investigate the dynamics of chemical reactions and how chemical structure influences electrical, magnetic, and optical properties. The creation of new computational methods and models to better understand molecular structures and chemical reactions is also an area of shared interest between the Chemical Sciences and Mathematical Sciences Divisions.

The Division's research portfolio will also reveal previously unexplored avenues for new Army capabilities while also providing results to support the ARL ERAs of (i) Implementation and (ii) Impact of Operating in a Contested Environment ERA. In addition, the Division supports the (i) the Materials Research Campaign's goals to create multifunctional, responsive materials, and to discover and exploit materials for more efficient power generation and energy storage, (ii) the Sciences-for-Maneuver Campaign's goals to identify and exploit innovations in energy sources, storage, and conversion, to discover novel materials to enable durable, damage tolerant structural systems, to discover materials to enable damage-tolerant structural systems, and to engineer and exploit chemical systems with biological-like functions for advanced protective equipment, and (iii) the Sciences for Lethality-and-Protection Campaign's goal to develop new energetic materials and predictive models of their behavior.

B. Program Areas

The Chemical Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the identification, evaluation and monitoring of research projects. In FY17, the Division managed research within these five Program Areas: (i) Polymer Chemistry, (ii) Molecular Structure and Dynamics, (iii) Electrochemistry, (iv) Reactive Chemical Systems, (v) Environmental Chemistry, and an International Program, (vi) Energy Transport and Storage. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Polymer Chemistry. The goal of this Program is to understand the molecular-level link between polymer microstructure, architecture, functionality, and the ensuing macroscopic properties. Research in this Program may ultimately enable the design and synthesis of functional polymeric materials that give the Soldier new and improved protective and sensing capabilities as well as capabilities not yet imagined. This Program is divided into two research thrusts: (i) Precision Polymeric Materials and (ii) Complex Adaptive Polymeric Systems.

The Precision Polymeric Materials Thrust supports research aimed at developing new approaches for synthesizing polymers with precisely-defined molecular weight, microstructure, architecture, and functional group location. Of particular emphasis are efforts that focus on novel methods for sequence and tacticity control in synthetic polymers as well as enabling the synthesis of novel 2D organic polymers. Also of interest are research efforts that explore how molecular structure influences polymer assembly into more complex, hierarchical structures and influence interactions with other materials (e.g., inorganic or biological materials) to render functional hybrid assemblies. The Complex Adaptive Polymeric Systems Thrust focuses on developing polymers that exhibit programmed molecular responses to external stimuli. In particular, the thrust emphasizes research efforts related to stimuli-responsive self-immolative polymers, polymer mechanochemistry, and stimuli-mediated polymer assembly. Additionally, research focused on exploring the assembly/incorporation of multiple responsive groups into a single polymeric material system as well as the incorporation of feedback mechanisms to engender complex responsive behavior is also of interest.

The research supported by this Program Area may lead to long-term applications for the Army such as light-weight, flexible body armor, materials for clothing that are breathable but also provide protection from toxins, and fuel cell membranes to harness renewable energy. In addition, the efforts in this program may ultimately lead to new, dynamic materials such as photohealable polymers that can be used as a repairable coating and mechanically- or thermally-responsive polymers and composites that can convert external forces to targeted internal chemical reactions (i.e., to convert external force to internal self-sensing and self-repair).

2. Molecular Structure and Dynamics. The goal of this Program Area is to understand state-selected dynamics of chemical reactions of molecules in gas and condensed phases across a wide variety of conditions, and to develop theories to accurately describing and predict these phenomena. In the long term, these studies may enable the design of future propellants, explosives, and sensors. This Program Area is divided into three Thrusts: (i) Molecular Dynamics, (ii) Quantitative Theoretical Methods, and (iii) Novel Energetic Materials.

The Molecular Dynamics Thrust supports research on the study of energy transfer mechanisms in molecular systems. The Quantitative Theoretical Methods Thrust supports research to develop and validate theories for quantitatively describing and predicting the properties of reactions and molecular phenomena. The Novel Energetic Materials Thrust supports research for the prediction, synthesis, and stabilization of novel energetic materials with order-of-magnitude gains in power and energy density over traditional C-H-N-O chemistries.

3. Electrochemistry. The goal of this Program Area is to understand the underlying science that controls reactant activation and electron transfer. These studies may provide the foundation for developing advanced power generation and storage technology. This Program Area is divided into two research Thrusts: (i) Reduction-oxidation (Redox) Chemistry and Electrocatalysis, and (ii) Transport of Electroactive Species.

The Redox Chemistry and Electrocatalysis thrust aims to discover spectroscopic and electrochemical techniques for probing surfaces and selected species on those surfaces, while the Transport of Electroactive Species thrust identifies and supports research to uncover the mechanisms of transport through polymers and electrolytes, to design tailorable electrolytes based on new polymers and ionic liquids, and explores new methodologies and computational approaches to study the selective transport of species in charged environments.

Research in this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications include the discovery and use of new mechanisms for the storage and release of ions that are potentially useful in future power sources, including new battery or bio-fuel concepts. In addition, studies of electroactive species may enable the development of multifunctional materials that simultaneously have ionic conductivity, mechanical strength, and suitable electronic conductivity over a considerable temperature range, while exposed to aggressive chemical environments.

4. Reactive Chemical Systems. The goals of this Program Area are to obtain a molecular level understanding of interfacial activity and of dynamic nanostructured and self-assembled chemical systems. High-risk basic research in this program is expected to lead to the design and synthesis of new chemical systems that will provide unprecedented hazardous materials management capabilities and soldier survivability. This Program Area is divided into two research Thrusts: (i) Interfacial Activity and (ii) Synthetic Molecular Systems. Within these thrusts, high-risk, high-payoff research is identified and supported to pursue the program's long-term goals.

The Interfacial Activity Thrust supports research on understanding the kinetics and mechanisms of reactions occurring at surfaces and interfaces and the development of new methods to achieve precise control over the structure and function of chemical and biological molecules on surfaces. Specific areas of interest include adsorption, desorption, and the catalytic processes occurring at surfaces and interfaces and the interface between nanostructures and biomolecules to generate advanced materials.

Research in the Synthetic Molecular Systems Thrust is exploring novel methods for incorporation of multi-functionality, stimuli-responsive, and dynamic behavior into chemical systems. Specific areas of interest include the stabilization of nanostructured and self-assembled systems, incorporation of enhanced catalytic activity into chemical systems, and the design and synthesis of chemical systems that sense and respond to specific stimuli.

This Program Area supports research that will likely lead to many long-term applications for the Army and the private sector. Potential long-term applications include novel chemical sensing capabilities, selective membranes, multi-functional surfaces for self-repair and self-healing, and new approaches to hazardous waste management. Research in these areas may also lead to multi-functional and stimuli-responsive systems for "smart" materials that can sense and autonomously respond in unprecedented ways for soldier protection.

5. Environmental Chemistry. The goal of this Program Area is to understand the fate and transport of chemicals in the environment. Research in this area is expect to provide a more complete and practical understanding of chemical pathways of degradation and transformation in the environment. The research will embrace environmental complexity by including the study of multiple phases and chemicals simultaneously present. Environmental surfaces of interest are soils (e.g., clay, sediments, dust), water (e.g., surface, snow) and films (e.g., biological and urban made). The program will identify fundamental research opportunities in two main Thrusts: (i) Chemical Fate and Transport, and (ii) Environmental Forensics.

The Chemical Fate and Transport Thrust supports research to uncover the mechanisms, thermodynamics and kinetics of chemical transport. Specific areas of interest include experimental and theoretical approaches to investigate sorption, degradation, and photo degradation mechanisms of chemical species under environmentally relevant conditions. Of particular interest is understanding the conditions that lead to degradation and transformation of contaminants, and develop novel speciation models of complex environmental media.

The Environmental Forensics Thrust focuses on developing integrated experimental and computational approaches to discern chemical transformation of contaminants from source to point-of-detection and provide predictions of its future transformations in different environments and conditions. This thrust also includes studies of the effect of manufacturing processes and the fate of chemicals released in the environment.

6. Energy Transport and Storage (International Program). As one of the ARO International Programs and part of the ARO Chemical Sciences Division portfolio, the Energy Transport and Storage Program Area is focused on supporting research at universities outside of the U.S., with the goal of building international partnerships and laying the foundational work upon which energy storage and power generation technologies depend. This program targets high-risk, fundamental research which addresses the core underlying limitations of energy transport/storage. Central to the mission of this program is the exploration of how materials and cell design can be tailored to enable targeted electrochemical reactions—while eliminating side reactions, hazards and other impediments, thereby surmounting hurdles and exploiting opportunities in chemical energy storage. This Program Area is divided into two research Thrusts: (i) Energy Transport and (ii) Thermal Energy Storage.

The Energy Transport Thrust supports research aimed at evaluation protocols for energy relevant materials and the scrutiny of new solid ion conductors and liquid/slurry active materials. There is a tendency to focus upon the most favorable aspects of energy-relevant chemistries and materials, but such reports often either fail to identify or neglect the key limiting characteristics which researchers in general and the Army in particular require to overcome the constraints which restrict breakthroughs in a given energy technology. Projects which actively seek to obtain a global understanding of the underlying principles regarding how chemicals/materials impact the stability and performance of energy storage technologies are of Army interest. Advances in solid electrolytes hold the promise of revolutionizing energy storage technologies, but numerous factors such as limited ionic conductivity, poor ion selectivity, high reactivity, composition changes during processing or difficult processing methods, high contact resistance, unfavorable mechanical properties, defect propagation during cycling due to mechanical deformation, cost barriers, etc. remain major obstructions to the integration of solid electrolytes/separators into devices. Innovative approaches to propel these critical cell components forward are sought. The identification of promising, new liquid (or slurry) active materials (*i.e.*, anolytes or catholytes) may potentially enable new cell designs which greatly simplify battery production, scalability and the tunable modularity of cells, thus enabling their assimilation into diverse Army-relevant energy storage applications.

The Thermal Energy Storage Thrust is focused on studies of thermal energy storage phase change materials (PCMs). PCMs permit both passive and active heating/cooling that can significantly reduce or eliminate the necessity of conventional heating and cooling methods (for buildings, refrigeration, electronics, etc.); however, applications are restricted due to their high cost, low thermal conductivity, change in density, limited stability of thermal properties and tendency to subcool. The discovery and characterization of new PCMs (e.g., based upon solvates) may overcome these challenges and provide a path forward for their widespread implementation.

C. Research Investment

The total funds managed by the ARO Chemical Sciences Division for FY17 were $55.3 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY17 ARO Core (BH57) program funding allotment for this Division was $9.2 million and $2.2 million of Congressional funds (T14). The DoD Multidisciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $10.1 million to projects managed by the Division. The Division also managed $17.9 million of Defense Advanced Research Projects Agency (DARPA) programs, and $1.9 million provided by other government agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $4.8 million for contracts. The Army's Institute for Soldier Nanotechnologies received $7.7 million. In addition, $1.8 million was provided for awards in the Historically Black Colleges and Universities and Minority Serving Institutions (HBCU/MSI) Programs, including funding for DoD-funded Partnership in Research Transition (PIRT), DoD-funded Research and Educational Program (REP) projects, and $0.3 million of the Division's ARO Core (BH57) funds, with the latter included in the BH57 subtotal above.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY17 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY17 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY17, the Division awarded 28 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Nicholas Abbott, University of Wisconsin - Madison; *New Principles for Targeting and Triggering based on Molecular Self-Assembly in Topological Defects of Liquid Crystals*
- Professor Saadyah Averick, Allegheny-Singer Research Institute; *Enhanced Enzymatic Catalysis in Organic Solvents - Taking Biology Out of the Cell and Into Chemical Synthesis*
- Professor Jovica Badjic, Ohio State University; *Commanding the Permeability and Stimuli-Responsive Characteristics of Vesicles/Polymersomes Composed of Dual-Cavity Baskets*
- Professor Adam Braunschweig, CUNY; *Donor-Acceptor Superstructures with Emergent Optoelectronic Properties: Synergistic Approaches to Functional Self-Assembling Aggregates*
- Professor Daniel Buttry, Arizona State University; *Anode And Electrolyte Calcium-Based Chemistries*
- Professor Phillip Christopher, University of California - Riverside; *Quantitative and Mechanistic Analyses of Bond Selective Chemistry via Non-Thermal Excitation of Metal Nanostructures*
- Professor Stephen Cronin, University of Southern California; *Hot Electron Injection in Photocatalytic Plasmon Resonant Nanostructures*
- Professor Suresh Dhaniyala, Clarkson University; *Characterization Of Aerosol Particle Charge As A Function Of Particle Size*
- Professor Barbara Finlayson-Pitts, University of California - Irvine; *Probing the Surfaces of Atmospheric Organic Particles*
- Professor Nathan Gianneschi, Northwestern University Evanston Campus; *Assembly and Dynamics of Soft Matter Observed by Liquid Cell TEM*
- Professor David Go, University of Notre Dame; Plasma-Induced Electrochemistry: *Understanding the Behavior of Electrons at a Plasma-Liquid Interface*
- Professor Andrew Herring, Colorado School of Mines; *Investigations of Anion Exchange Polymer Interfacial Interactions*

- Professor Patrick Howlett, Deakin University (Australia); *Design Of High Ion Conductivity In Polymer/Oipc Composite Through Understanding The Effect Of Chemistry On Structure And Ion Dynamics*
- Professor Stephen Klippenstein, University of Chicago; *Theoretical Kinetics Driven Mechanism Development for the Combustion of Rocket and Gun Propellants*
- Professor Svetlana Kotochigova, Temple University; *Effect Of Conical Intersections On Chemical Reactivity Of Ultracold Molecules In Optical Potentials*
- Professor Dongxia Liu, University of Maryland - College Park; *Multi-functional Ultra-thin Film Photocatalytic Light Absorber*
- Professor Douglas MacFarlane, Monash University (Australia); *Organic Salts as Intermediate Phase Change Materials*
- Professor Daniel Mackowski, Auburn University; *Modeling of Ultraviolet Optical Intensities in Agglomerates of Spores and Vegetative Cells Exposed to Sunlight*
- Professor John Morris, Virginia Polytechnic Institute & State University; *Photocatalytic Epoxidation Of Propene: Fundamental Studies Of Uptake, Binding, And Reaction Mechanisms*
- Professor Ryan O'Hayre, Colorado School of Mines; *Triple Conducting Oxides for Electrochemical Energy Conversion and Storage*
- Professor Dmitrii Perepichka, McGill University; *2D Conjugated Polymers from Stable Free Radical Building Blocks*
- Professor Timothy Strobel, Carnegie Institution of Washington; *Rationally Designed Materials Through Kinetically Controlled Synthesis*
- Professor Arthur Suits, University of Missouri - Columbia; *Quantum Aspects of Roaming Radical Reactions*
- Professor Veronica Vaida, University of Colorado - Boulder; *Chemical Micro Reactors in the Environment*
- Professor Lauren Webb, University of Texas - Austin; *Developing Adaptable Models for Studying Fundamental Properties of Immobilized Enzymes*
- Professor Peter Weber, Brown University; *Ultrafast Chemical Dynamics on Complex, Excited State Energy Landscapes*
- Professor Choong-Shik Yoo, Washington State University; *Dense Carbon-Organic Framework Solids in High Energy Density*
- Professor Gleb Yushin, Georgia Tech Research Corporation; *Electrochemical Reactions of Metal Fluorides with Lithium-ion Electrolytes in Carbon Nanopores*

2. Short Term Innovative Research (STIR) Program. In FY17, the Division awarded 6 new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Patrick Cappillino, University of Massachusetts - North Dartmouth; *Multifunctional, Bimetallic Nanomaterials Prepared by Atomic Layer Electroless Deposition*
- Professor Robert Counce, University of Tennessee - Knoxville; *Enabling Science for Redox Flow Batteries based on Room Temperature Ionic Liquids*
- Professor Mark Mirotznik, University of Delaware; *3D Printing of Metal Oxide Framework Materials*
- Professor Charles Mullins, University of Texas - Austin; *UHV Surface Science Investigations of Adsorption, Reaction and Diffusion in Ultra-thin Metal Organic Framework Films*
- Professor Eugene Smotkin, Northeastern University; *An Operando Confocal Micro-Raman Spectroscopy Cell For Intermediate Temperature MIEC Membrane Development*
- Professor Bobby Wilson, Texas Southern University; *Canonical Tensors Applied to Ab Initio Electronic Structure: Linear Scaling for Metallic Systems*

3. Young Investigator Program (YIP). In FY17, the Division awarded two new YIP projects to drive fundamental research in areas relevant to the current and future Army. The following PIs and corresponding organizations were awarded the new-start YIP project.

- Professor Kevin Leonard, University of Kansas; *Development of a 'Macro' SI-SECM Protocol to Investigate Reaction Intermediates*
- Professor Joshua Sangoro, University of Tennessee - Knoxville; *Decoupling Of Ionic Conduction From Structural Dynamics In Polymerized Ionic Liquids*

4. Conferences, Workshops, and Symposia Support Program. The Division provided funds in support of a range of scientific conferences, workshops, and symposia that were held in FY17. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences, with the goal of supporting scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army, and to define the research needs, thrusts, opportunities, and innovation crucial to the future Army. Proposals requesting funding support, typically for less than $10K, were received and evaluated in line with the publicly available ARO BAA. In FY17, sixteen proposals were selected for funding by the Division to support FY17 conferences, workshops, or symposia.

5. Special Programs. In FY17, the Division also awarded eight new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school and undergraduate students. These efforts were funded through the ARO Core Program and Youth Sciences Programs, for research to be performed at academic laboratories currently supported through active SI awards (refer to CHAPTER 2, Section IX).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These projects constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Ion Transport in Complex Organic Materials. This MURI began in FY10 and was awarded to a team led by Professor Andrew Herring at the Colorado School of Mines. This MURI team investigated the interplay of chemical processes and membrane morphology in anion exchange, with the project ending in FY17.

Ion transport in complex organic materials is essential to many important energy conversion approaches. Unfortunately, ion transport is poorly understood in terms of its relationship to water content, morphology, and chemistry. While a great deal of research has focused on proton exchange membranes, little work has been performed with anion exchange membranes. This MURI team explored the fundamentals of ion transport by developing new polymer architectures (*e.g.*, polymer membranes) using standard and novel cations. These new polymer architectures and aqueous solutions containing representative cations served as a model system for studies of anion transport and its relationship to polymer morphology. In the longer term, the design and synthesis of robust, thin alkali-exchange membranes, combined with an improved understanding of ion exchange gained through the characterization of these membranes, could enable the development of new classes of fuel cells. Based on the MURI team's characterization of the fundamental processes of ion exchange across these polymer membranes, future fuel cells using similar membranes could harness alkali exchange, resulting in inexpensive, durable, and flexible-source power for the Army and commercial use.

2. Peptide and Protein Interactions with Abiotic Surfaces. This MURI began in FY11 and was awarded to a team led by Professor Zhan Chen at the University of Michigan, Ann Arbor. This MURI is exploring the processes that occur at biological/abiological interfaces. This research is co-managed by the Chemical Sciences and Life Sciences Divisions.

The objective of this research is to develop a systematic understanding of biological/abiological interfaces and how to design systems for predicted biological structure and function. The MURI team is using a combination of modeling and experimental techniques to understand the interactions of peptides and proteins covalently immobilized on abiotic surfaces. Specifically, the team will be investigating two peptides and one enzyme, with a variety of surfaces, such as self-assembled monolayers, chemically functionalized liquid crystalline films, and chemical vapor deposited polymers. The immobilized biological species will be characterized to determine not only structure but also activity. The investigators will utilize systematic modifications of the surface to probe the effect of chemical composition, morphology, and hydrophobicity on biological structure and function. The role of water will also be probed to determine how hydration affects not only immobilization, but also structure and function. Results from this research may ultimately enable the incorporation of nanostructured abiotic/biotic materials in applications such as sensing, catalysis, coatings, drug delivery, prosthetics, and biofilms.

3. High-Resolution Quantum Control of Chemical Reactions. This MURI began in FY12 and was awarded to a team led by Professor David DeMille at Yale University. This MURI is exploring the principles of ultracold molecular reaction, where chemical reactions take place in the sub-millikelvin temperature regime. This research is co-managed by the Chemical Sciences and Physics Divisions.

The study of ultracold molecular reactions, where chemical reactions take place in the sub-millikelvin temperature regime, has emerged as a new field in physics and chemistry. Nanokelvin chemical reactions are radically different than those that occur at “normal” temperatures. Chemical reactions in the ultracold regime can occur across relatively long intermolecular distances, and no longer follow the expected (Boltzmann) energy distribution. The reactions become heavily dependent on nuclear spin orientation, interaction strength, and correlations. These features make them a robust test bed for long-range interacting many-body systems, controlled reactions, and precision measurements.

The objectives of this MURI are to develop a fundamental understanding of the nature of molecular reactions in the nanokelvin temperature regime and to extend the cooling technique previously demonstrated by Professor DeMille[1] (through a previous ARO award) to other molecular candidates. The researchers will focus will be on the implementation of novel and efficient laser cooling techniques of diatomic molecules, and to understand the role of quantum effects, including the role of confined geometries, on molecules that possess vanishingly-small amounts of thermal energy. This research could ultimately lead to new devices or methods that explicitly use quantum effects in chemistry, such as the precision synthesis of mesoscopic samples of novel molecular compounds, new avenues for detection of trace molecules, and a new understanding of combustion and atmospheric chemical reactions.

4. Coherent Effects in Hybrid Nanostructures. This MURI began in FY12 and was awarded to a team led by Professor Naomi Halas at Rice University. This MURI is investigating nanomaterials and how these materials can control the propagation of electromagnetic (EM) energy.

Fundamental research involving metamaterials, quantum dots, plasmonic nanostructures, and other materials systems during the last decade has demonstrated the unique ability to selectively and actively control and attenuate electromagnetic energy from the far infrared through ultraviolet regions. The absorption frequency is dependent on shape, size, orientation, and composition of the nanomaterial. The nanoparticles act as antennae that redirect, focus or otherwise re-radiate the incoming energy. Because this is a resonance phenomenon, the media is generally transparent over a broad frequency range, with one or more resonances that absorb at specific frequencies. A goal in the control of the propagation of EM energy is the design of a material that absorbs over a broad frequency range and is transparent at one or more specific frequencies.

The objective of this research is to develop a fundamental understanding of nanomaterials to control the propagation of EM energy, with a particular emphasis on designing and investigating materials that have a broad spectrum absorption with a narrow, selective window of transmission. The MURI team is using a combination of computational, nanoscale fabrication, and characterization techniques to tailor electromagnetic properties for materials in specific, selected regions of the spectrum. The research team is focusing on designing, synthesizing, and combining nanoparticles and nanoparticle-based complexes to yield nanocomplexes exhibiting optimized coherent effects. This research may ultimately enable the design of materials with precisely-positioned transparency or absorbency windows that will impact Army applications in broadband scattering and absorption.

[1] Shuman ES, Barry JF, DeMille D. (2010). Laser cooling of a diatomic molecule. *Nature*. 467:820–823.

5. Theory and Experiment of Cocrystals: Principles, Synthesis and Properties. This MURI began in FY13 and was awarded to a team led by Professor Adam Matzger of the University of Michigan at Ann Arbor. This MURI team is investigating molecular co-crystal formation and the implications for controlling solid-state behavior. This research is co-managed by the Chemical Sciences and Materials Science Divisions.

The largely untapped potential for creating new molecular crystals with optimal properties is just beginning to be realized in the form of molecular co-crystallization. Co-crystallization has the potential to impact the macro-scale performance of many materials, ranging from energetic materials, to pharmaceuticals, to non-linear optics. Unfortunately, the dynamics of molecular co-crystal formation is poorly understood. Molecular co-crystals contain two or more neutral molecular components that rely on non-covalent interactions to form a regular arrangement in the solid state. Co-crystals are a unique form of matter, and are not simply the result of mixing two solid phases. Organic binary co-crystals are the simplest type and often display dramatically different physical properties when compared with the pure 'parent' crystals. A significant amount of research on co-crystal design has been carried out by the pharmaceutical industry for the synthesis of pharmaceutical ingredients. However, co-crystal design has not been exploited in broader chemistry and materials science research areas. A recent breakthrough discovery demonstrates that co-crystallization can be used to generate novel solid forms of energetic materials.

The objective of this MURI is to develop a fundamental understanding of intermolecular interactions in the context of crystal packing, and to use the knowledge gained for the design of new co-crystalline molecular materials with targeted, optimized physical and chemical properties. In the long term, a better understanding and control of molecular co-crystallization has the potential to improve the properties of a variety of materials, including: energetic materials, pharmaceuticals, organic semiconductors, ferroelectrics, and non-linear optical materials.

6. Artificial Cells for Novel Synthetic Biology Chassis. This MURI began in FY13 and was awarded to a team led by Professor Neal Devaraj at the University of California - San Diego. The goal of this MURI is to understand how biological and biomimetic synthetic cellular elements can be integrated to create novel artificial cells with unprecedented spatial and temporal control of genetic circuits and biological pathways. This research is co-managed with the Life Sciences Division.

The field of synthetic biology aims to achieve design-based engineering of biological systems. Toward this goal, researchers in the field are identifying and characterizing standardized biological parts for use in specific biological organisms. These organisms serve as chassis for the engineered biological systems and devices. While single-celled organisms are typically used as synthetic biology chassis, the complexity of even these relatively simple organisms presents significant challenges for achieving robust and predictable engineered systems. A potential solution is the development of minimal cells which contain only those genes and biomolecular machinery necessary for basic life. Concurrent with recent advances toward minimal biological cells, advances have also been made in biomimetic chemical and material systems, including synthetic enzymes, artificial cytoplasm, and composite microparticles with stable internal compartments. These advances provide the scientific opportunity to explore the integration of biological and biomimetic elements to generate an artificial hybrid cell that for the first time combines the specificity and complexity of biology with the stability and control of synthetic chemistry.

The objective of this MURI is to integrate artificial bioorthogonal membranes with biological elements to create hybrid artificial cells capable of mimicking the form and function of natural cells but with improved control, stability, and simplicity. If successful, these artificial cells will provide a robust and predictable chassis for engineered biological systems, addressing a current challenge in the field of synthetic biology that may ultimately enable sense-and-respond systems, drug-delivery platforms, and the cost-effective production of high-value molecules that are toxic to living cells (e.g., alternative fuels, antimicrobial agents).

7. Attosecond Electron Dynamics. This MURI began in FY14 and was awarded to a team led by Professor Stephen Leone at the University of California - Berkeley. The goal of this MURI is to use attosecond light pulses to study the electron dynamics of atoms and small molecules. This research is co-managed with the Physics Division.

Attosecond dynamics is a new field of scientific investigation which allows one to examine dynamics phenomena on the natural timescale of electronic processes in atoms, molecules, and materials. The timescale of microscopic dynamics in quantum systems occur at a timescale about one order of magnitude less than those for less-energetic processes, such as valence electronic transitions in molecules and semi-conductor materials. A recent scientific breakthrough known as double optical gating has led to the production of broadband laser pulse widths as short as 67 attoseconds, making direct observation of a variety of electronic phenomena possible in real time. Thus, now there exist opportunities to examine a variety of electron-dynamics phenomena that arise from electronic motions in molecules on the attosecond timescale.

The objective of this research is to harness attosecond pulses of electromagnetic energy to probe matter (e.g., atoms, molecules, plasmas) at attosecond time scales for the real-time observation, control, and understanding of electronic motion in atoms, molecules, and materials. If successful, this research may lead to new synthesis methods, such as plasmonically-enhanced catalysis for the direct reduction of CO_2 to create fuels, new schemes and manufacturing methods for solar photovoltaics, nano-catalysts for fuel combustion, and high-density specific impulse propellants.

8. Multistep Catalysis. This MURI began in FY14 and was awarded to a team led by Professor Shelley Minteer at the University of Utah. The goal of this MURI is to enable multi-step chemical reactions through the rational design of architectures that control the spatial and temporal pathways of precursors, intermediates, and products. This research is co-managed with the Materials Science Division.

The Krebs cycle is an exquisite example of a regulated enzyme cascade which biological systems use to precisely control charge and reactant transport to produce energy for the cell. Conversely, man-made systems typically involve a series of conversions with intermediate purification steps to achieve a desired product, with yield losses that compound with each step. The current approach to achieve multi-step reactions in a single reactor is an arbitrary combination of multiple catalysts that is likely to lead to poor yield with unreacted intermediates or byproducts of reactants that have reacted with the incorrect catalysts. Recent breakthroughs in materials synthesis, such as self-assembly and lock-and-key type architectures, offer control of surface arrangement and topology that enable a much more effective approach to achieving multi-step reactions through control of spatial and temporal transport of reactants, electrons, intermediates, and products.

The objective of this research is to establish methodologies for modeling, designing, characterizing, and synthesizing new materials and structures for the design and implementation of multi-step catalysis. In particular, integrated catalytic cascades will be created from different catalytic modalities such that novel scaffolding and architectures are employed to optimize selectivity, electron transfer, diffusion, and overall pathway flux. If successful, this research will provide unique paradigms for exploiting and controlling multistep catalysis with dramatically enhanced efficiency and complexity. In the long term, the results may lead to new energy production and storage technologies.

9. Multi-Scale Responses in Organized Assemblies. This MURI began in FY16 and was awarded to a team led by Professor Sankaran Thayumanavan, at University of Massachusetts - Amherst. The goal of this MURI is to understand how a molecular level detection can be propagated across a macroscopic material to affect a global property change that spans multiple length and time scales, and connecting these multi-scale events to realize signal amplification. This research is co-managed with the Materials Science Division.

Living systems are complex systems capable of receiving and using information, interacting with each other and their environment, and performing specific functions in response to stimuli occurring at multiple length and time scales. These sophisticated, innate behaviors are essential for survival, and can be extremely valuable in non-natural systems. A variety of synthetic systems have been engineered to respond to specific stimuli; however, the dynamics of the chemical and material processes and interactions occurring at multiple length and time scales throughout the signal-propagate-response pathway are inadequately understood to rationally design autonomous, "living" systems. The daunting challenge toward synthetic "living" systems is predictably propagating a molecular level change, generated through the selective sensing of a trigger, into a readily discernible macroscopic change in a material's fundamental properties. This can only be addressed by developing a fundamental understanding of the chemical processes that occur at multi-scale levels – from molecular to nano to macroscopic length scales and from nanoseconds to hours. The inherent complexity involved in connecting these length scales, and the propagation and amplification of the resulting signals, requires a cohesive, multidisciplinary approach.

The integrated research plan led by Professor Thayumanavan is comprehensive and addresses each of the key elements needed to understand the fundamental multi-scale responses of adaptive systems occurring across length and time scales. The research is exploiting a variety of material platforms/approaches, including liquid crystal orientation, responsive amphiphiles, depolymerization, and biological/abiological composites with non-equilibrium molecular release to address propagation and amplification at multiple length scales. Each system approach is innovative, well-formulated, and focused on a complete understanding of the basic research principles controlling each approach. A variety of triggers will be considered throughout the effort including pH, temperature, redox, light, and enzymes. A key part of this effort is the ability to monitor dynamic changes during the cooperative reorganization processes at the interface, and this is addressed by integration of novel characterization techniques such as in situ liquid cell transmission electron microscopy. If successful, this fundamental research may ultimately enable Army-relevant technologies in stimuli-responsive systems such as self-decontaminating materials, controlled release for hazardous materials management or drug delivery, and responsive systems for self-healing and smart materials.

10. Sequence-Defined Synthetic Polymers Enabled by Engineered Translation Machinery. This MURI began in FY16 and was awarded to a team led by Professor Michael Jewett at Northwestern University – Evanston. The goal of this MURI is to engineer the translation machinery to accept and polymerize non-biological monomers in a sequence-defined manner using non-traditional chain growth polycondensation chemistries (beyond amide and ester linkages). This research is co-managed by the Chemical Sciences (lead) and Life Sciences Divisions.

Employing only four nucleotides and twenty amino acids, a plethora of biopolymers (e.g., proteins, DNA) with precisely-defined building block sequence gives these materials the ability to fold into higher-ordered structures capable of performing a variety of advanced functions such as information storage, self-replication, and signal transduction. The ability to extend comparable molecular-level sequence control to synthetic polymers, which have a much wider range of monomeric building blocks, has many scientific and technological implications, as it would enable precise control over structure-property relationships. Recent work has demonstrated that altering the sequence of short conjugated phenylene-vinylene oligomers can significantly modulate both electronic and optical properties. While greater complexity in function is anticipated for longer chain sequence-defined polymers, chemical routes to their synthesis have remained elusive. Conversely, biology synthesizes long sequence-defined polymers with extremely high efficiency and accuracy by employing templates to provide sequence information. More specifically, the ribosome, the workhorse of the translation machinery, is very adept at sequence-defined polymer synthesis through the successive condensation of amino acids (monomers), but primarily performs a single type of chemistry—amide bond formation via a chain-growth condensation polymerization. Co-opting the natural translation machinery to accept non-biological monomers is an attractive approach to synthesize non-biological polymers with the sequence control of biology. However, this approach is limited by cell viability constraints; thus, in vitro engineering of the translation machinery may offer unprecedented freedom of design to modify and control ribosome chemistry.

The objective of this research is to engineer and repurpose the translation apparatus (including the ribosome and the associated factors needed for polymerization) to produce new classes of sequence-defined polymers. In the long term, this research may enable a broad range of disruptive technologies having significant impact on DoD capabilities. Sequence control at the atomic level will give the greatest possible control over the emergent, macroscopic behavior of oligomers and polymers, leading to new advanced personal protective gear, sophisticated electronics, fuel cells, advanced solar cells, and nanofabrication, which are all key to the protection and performance of soldiers.

11. Multi-modal Energy Flow at Atomically Engineered Interfaces. This MURI began in FY16 and was awarded to a team led by Professor Jon Paul Maria of the North Carolina State University. The objective of this MURI is to bring chemistry, materials, surface science, electrochemistry, and physics together to characterize and understand short time-frame sub-nanoscale non-equilibrium phenomenon at and across materials interfaces, especially the flow, redistribution and partition of energy near the interface by devising and applying novel experimental, theoretical, and simulation approaches. This research is co-managed between the Mechanical Sciences (lead) and Chemical Sciences Divisions.

The MURI team approach will be to explore, identify, and define multiple mechanisms of energy transfer/transduction at precision-engineered interfaces. Material systems that support energy transfer through lattice/molecular vibrations, plasmon-electron coupling, and chemical reactions will be studied. The synthesis, measurement, and modeling activities are co-designed to promote extreme-non-equilibrium excitations within nano-scale geometries; to observe in situ picosecond to microsecond property responses using newly developed methods; to inform new theoretical models; and to enable accurate multiscale prediction. The plan of work explores a simple, overarching, and materials-generic hypothesis: function and failure in advanced functional materials are overwhelmingly affiliated with interfaces, where the underlying mechanisms (desirable and undesirable) are regulated by or related to energy transfer/ transduction among inhomogeneous boundaries. Observing and understanding the local processes over multiple time and length scales will improve existing and design new materials systems, and to predict their performance.

12. Adaptive Self-assembled Systems. This MURI began in FY17 and was awarded to a team led by Professor Anna Balazs of the University of Pittsburgh and is being jointly managed by the Materials Science and the Chemical Sciences Divisions. The goal of this effort is to develop experimental and theoretical approaches to integrate microscopic forms of self-organization with a scalable means of additive 3D fabrication.

Recent research related to the bottoms-up assembly of material has demonstrated the feasibility of using tailored short-range interactions to drive the assembly of functional clusters and macromolecular assemblies that are capable of performing basic functions such as catalysis, energy harvesting, color change and actuation. However, it is not currently possible to go beyond basic functionality and establish hierarchically ordered systems that display complex functional integration and dynamic system response. In particular, multifunctional structures with specifically targeted properties and robust feedback and control mechanisms that can embody aspects of emergent behavior and robust reconfiguration remain well beyond reach. This effort aims to establish the knowledge and expertise base needed to enable the design and directed assembly of nano-building blocks into complex, hierarchical 3D architectures capable of long-range control over multifunctional behavior and smart/dynamic responses using an additive 3D material assembly approach. The research is organized around three major thrusts: (i) assembly of microscale musculoskeletal frameworks, (ii) transduction of energy to enable functionality, and (iii) additive manufacturing of large-scale dynamic material systems. If successful, the research will enable the development of artificial "smart" materials and structures that exhibit tightly coupled capabilities for sensing environmental cues and then transducing energy to perform useful, situation-specific dynamic responses.

C. Small Business Innovation Research (SBIR) – New Starts

Research within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. The Division managed nine new-start SBIR contracts in FY17, in addition to managing active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY17 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY17, the Division managed eleven new-start STTR contracts, in addition to active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of STTR topics published in FY16 and a list of prior-year topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Serving Institutions (HBCU/MSI) – New Starts

The HBCU/MSI program encompasses the (i) Partnership in Research Transition (PIRT) Program awards, (ii) DoD Research and Educational Program (REP) awards for HBCU/MSI, and (iii) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY17, the Division managed four new REP awards, in addition to active projects continuing from prior years. In addition, proposals from HBCU/MSIs are often among the projects selected for funding by the Division (refer to the list of HBCU/MSI new starts in *CHAPTER 2, Section IX*.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The following PECASE recipient, previously nominated by this Division, was announced in this fiscal year by the White House. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Stabilization of Reactive Chemical Species and Fundamental Studies of Small-Molecule Reactivity in Metal-Organic Frameworks. The objective of this PECASE, led by Professor Thomas Harris and Northwestern University is to design and synthesize porphyrin containing metal-organic frameworks (MOFs) and determine their stability and reactivity in catalytic transformations, as well as their ability to stabilize small reactive molecules.

This PECASE award will expand on studies initiated as part of a prior YIP project led by the same investigator. This effort will provide a comprehensive understanding of the stability and reactivity of iron porphyrin containing MOFs. This work will provide a unique method for the stabilization of highly reactive oxo and nitrogen containing species. These multifunctional materials have potential applications for the Army in decontamination, sensing, soldier protection, and self-responding materials.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY17, the Division managed nine new DURIP projects, totaling $1.5 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. University Affiliated Research Center (UARC): Army Institute for Soldier Nanotechnologies (AISN)

The AISN, located at the Massachusetts Institute of Technology (MIT), carries out fundamental, multidisciplinary, nanoscience research that is relevant to the Soldier. Nanoscience research creates opportunities for new materials, properties, and phenomena as material properties (*e.g.*, color, strength, conductivity) become size dependent below a critical length scale of about 100 nanometers. The research performed at the AISN falls into three Strategic Research Areas (SRAs): (i) Lightweight, Multifunctional Nanostructured Materials (ii) Soldier Medicine, and (iii) Blast and Ballistic Threats. Each SRA is further divided into research themes. Detailed descriptions of each SRA and its corresponding themes are available at the AISN program website (http://mit.edu/isn/research/index.html).

In FY17, the AISN supported 25 faculty, 60 graduate students, and 25 postdoctoral fellows across 14 departments at MIT. The AISN program is unique in that it currently has 10 industrial partners positioned to receive promising technical results and work to bring new products and capabilities to the Soldier, as well as a mechanism for additional industry partners to join and leave the Institute, depending on needs and activities. A U.S. Army Technical Assessment Board and an Executive Steering Board biannually review the AISN research portfolio, assessing the goals of the various projects and research results. The AISN and its industry partners are well-situated to perform basic and applied research in response to Soldier needs now and in the future. A total of $7.7 million of program funds was allocated to the AISN in FY17, which was the fifth year of a contract that was renewed in FY12 for a five-year period. Of these FY17 funds, $5.3 million was allocated for 6.1-basic research and $1.6 million was allocated for five applied-research projects.

I. DARPA Agnostic Compact Demilitarization of Chemical Agents (ACDC) Program

DARPA's Agnostic Compact Demilitarization of Chemical Agents (ACDC) program is exploring new technologies for neutralization of bulk stores of chemical warfare agents (CWAs) and organic precursors at or near the site of storage. ACDC is developing and demonstrating the technologies needed to construct a transportable, prototype system that converts organic compounds into constitutive carbon/nitrogen/phosphorous/sulfur oxides and stable alkali or alkaline earth metal salts, or another demonstrated safe form. A final ACDC system would feature chemistries for agent destruction and sequestration of halogens and other components using locally available resources. ARO is providing subject matter expertise and an ARO program manager is serving as the COR on the awarded efforts.

J. DARPA Make-It Program

The DARPA Make-It program aims to address these challenges by developing technologies to accelerate chemical discovery and production beyond conventional batch-based capabilities by exploiting continuous synthetic approaches. The goal of Make-It is to develop a fully automated chemical synthesizer that can produce, purify, characterize and scale a wide range of small molecules. Make-It systems would likely include components for knowledge-based computational tools for reaction pathway prediction; algorithms for automation and process control; and interconnected fluidic modules for continuous synthesis, in-line characterization, purification and formulation. If realized, such a system would not only speed the pace of chemical innovation and small-molecule manufacturing, but would also provide an accessible chemical synthesis platform for non-specialists. ARO is providing subject matter expertise and an ARO program manager is serving as the COR on the awarded efforts.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Chemical Sciences Division.

A. Chemical transformations via photon induced metal-to-molecule electron transfer

Professor Phillip Christopher, University of California, Riverside, YIP

The goal of this research was to develop insights into approaches for controlling catalytic processes through direct photoexcitation of adsorbate metal bonds. This was highlighted in collaborative work performed during FY17 where the efficiency of various photocatalytic processes was compared with the same (and different) photocatalysts. It was observed that an identical photocatalyst could exhibit different wavelength dependent efficiencies as a function of reaction, providing evidence that there is specificity in how photon energy is transferred to molecules (see FIGURE 1). In addition, the team answered questions raised from work performed earlier in this project associated with how adsorbates restructure catalytic materials by combining *in-situ* microscopy, spectroscopy and theoretical calculations (see FIGURE 2).

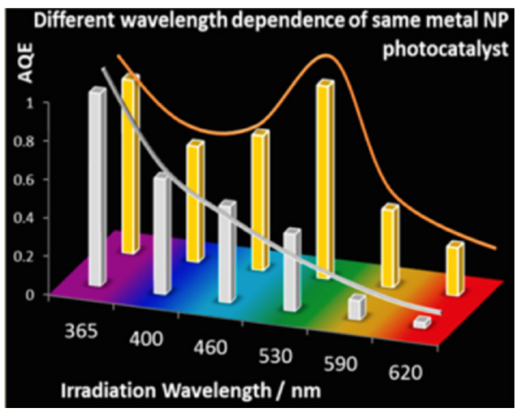

FIGURE 1

Comparison of efficiency of various photocatalytic processes with the same (and different) photocatalysts. An example of how the wavelength dependent photocatalytic reaction efficiency could change for the same catalyst, but different reaction. Adapted from *J. Phys. Chem. Lett.* 2017, 8, 2526−2534.

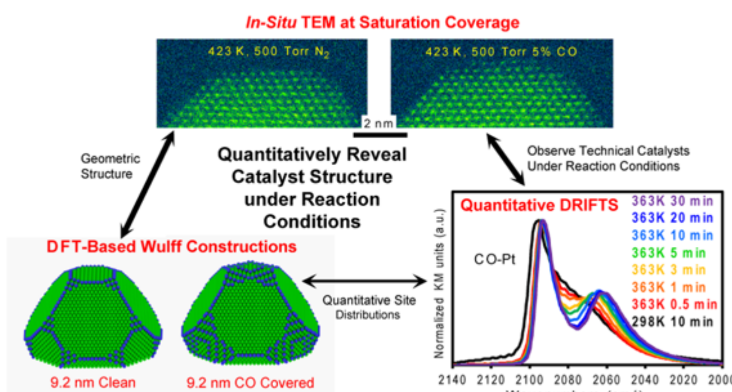

FIGURE 2

Reconstruction of Pt nanoparticles. The panels provide a schematic of how *in-situ* microscopy, spectroscopy and theory were used to understand the reconstruction of Pt nanoparticles by the adsorption of CO. Adapted from *J. Am. Chem. Soc.*, 2017, *139*, 4551–4558.

B. Tracking Living Polymerization at the Single-Molecule Level
Professor Peng Chen, Cornell University, Single Investigator Award

Catalytic polymerization is a key process in making synthetic polymers. In chain-growth polymerization, a chain grows from a catalyst continually to reach thousands of subunits. However, the real-time dynamics of chain growth remains unknown. The objective of Professor Chen's research is to develop novel single-molecule approaches to visualize the growth of individual polymers, so as to understand their real-time growth dynamics and how this dynamics affects polymer properties.

In FY17, research efforts led to the successful development of a magnetic tweezers based approach to visualize real-time polymer growth at the single-polymer level. The research team focused on ring-opening metathesis polymerization and found that the extension of a growing polymer under a pulling force does not increase continuously but exhibits wait-and-jump steps, which is a first-of-its-kind discovery (see FIGURE 3). These steps are attributable to the formation and unraveling of conformational entanglements from newly incorporated monomers during nonequilibrium living polymerization, whose presence was previously unkonwn. Combining the experiments with molecular dynamics simulations, the team also found that the configurations of these entanglements play a key role in determining the polymerization rates and the dispersion among individual polymers, opening new opportunities to manipulate polymer conformation during synthesis. Results from this research were recently published in *Science*, highlighted in *Science*, *Nature*, and *Chemical & Engineering News*, and selected as an example of "Research of the Year" by *Chemical & Engineering News*.

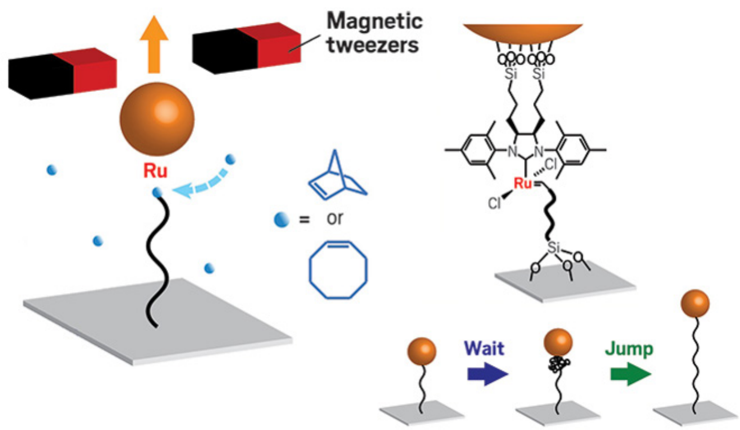

FIGURE 3

Real-time visualization of a ring-opening polymerization. These studies revealed previously unknown wait-and-jump steps due to the formation and unraveling of conformational entanglements from newly incorporated monomers.

C. New Understanding of Surface Bonding through High Speed Imaging
Professors Keith Nelson and Christopher Schuh, Massachusetts Institute of Technology, AISN (UARC)

This research, led by investigators at the Army's Institute for Soldier Nanotechnologies (AISN), aims to understand materials physics under impact. The notion of impact-induced adhesion has been implemented in powder processing through kinetic deposition or cold spray. Kinetic deposition has proven successful in making coatings, in reclaiming damaged metallic surfaces, and in additively manufacturing bulk metallic materials. In the same school of thought, localized melting has been generally perceived as an advantage, if not the main mechanism, for the adhesion of metallic microparticles to substrates during a supersonic impact.

In FY17, the research team has demonstrated the first in situ supersonic impact observations of individual metallic microparticles aimed at the explicit study of melting effects. Counterintuitively, researchers found that under at least some conditions melting is disadvantageous and hinders impact-induced adhesion (see FIGURE 4). In the parameter space explored, i.e., ~10 µm particle size and ~1 km/s particle velocity, researchers showed that the solidification time is much longer than the residence time of the particle on the substrate, so that resolidification cannot be a significant factor in adhesion.

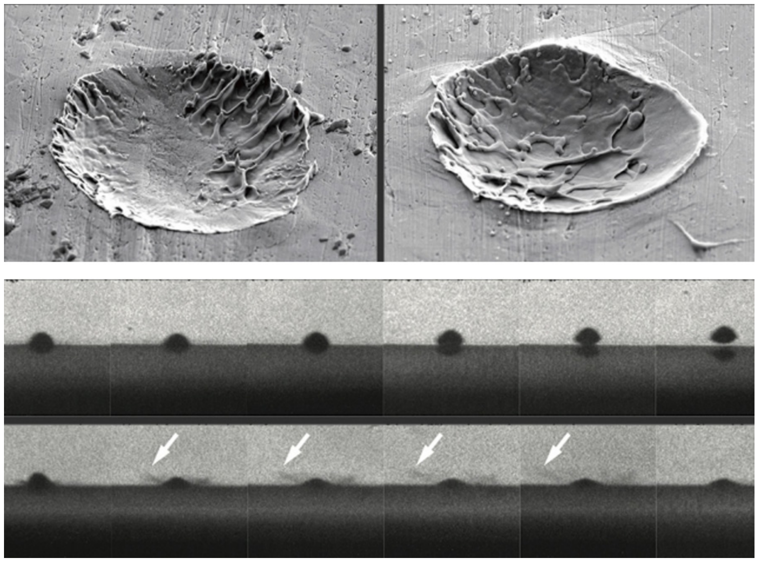

FIGURE 4

SEM and *In Situ* observation of microparticle supersonic impact. Micrograph of a metal surface after impact by Al microparticles. Creaters are formed due to melting of the surface from the impact. Even though the substrate melted at increasing impact velocities, melting clearly did not lead to adhesion (top right/left). Multiframe sequences with 5 ns exposure times showing 15-μm Al particle impacts on a Zn substrate and Al substrate at 940 and 950 m/s, respectively, impact velocity. The microprojectile arrives from the top of the field of view. It rebounds after impacting on Zn but adheres to Al (bottom row).

D. SFG Spectroscopy of the Graphene/Water Interface

Professors Stephen B Cronin and Alex Benderskii, University of Southern California

The goal of this research is to use vibrational sum frequency generation (vSFG) spectroscopy to characterize molecules in solution under various electrochemical conditions as a function of electrochemical potential and electrolyte. The research team successfully measured the voltage dependence of the SFG spectra of the graphene/D_2O interface taken under various applied electrochemical potentials (see FIGURE 5). The team found that hydrogen-bonded peaks (2350 and 2500 cm^{-1}) increase with increasing voltage while the free-OD peak (2700 cm^{-1}) remains unchanged in intensity. When examining the free-OD peak, researchers found a blue-shift with increasing voltage. This shift is due to the Stark shift of the molecule, which provides a measure of the electric field at the electrode surface, reaching a magnitude of 0.1 V/Å. These results agree well with theoretical predictions and validate this approach as an interesting new way to probe reactions at electrochemical surfaces.

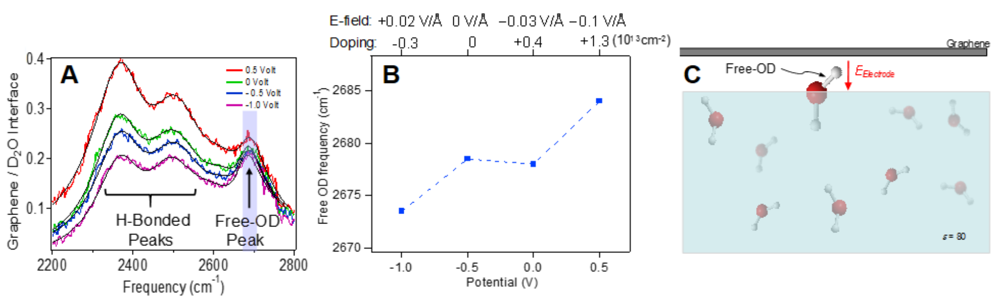

FIGURE 5

Voltage dependence of the SFG spectra of the graphene/D_2O interface. (**A**) SFG spectra of the D_2O/graphene interface under various applied potentials. (**B**) Free-OD vibrational frequency plotted as a function of applied potential showing a clear Stark shift of 10 cm^{-1}. The carrier concentration in the graphene (obtained from the *G* band Raman shift) and electric field are also indicated. (**C**) Schematic diagram illustrating the D_2O/graphene interface. The free-OD peak corresponds to the topmost water (or D_2O) molecule at the electrode surface, whose OD bond sticks out of the solution and is therefore not H-bonded. The change in the H-bonded peak intensities reflect changes in the thickness of the Debye layer with voltage (i.e., local ion concentration)

E. Bio-Inspired Design of Adaptive Catalysis Cascades

Professor Shelley Minteer, University of Utah, MURI Award

Enabling multi-step chemical and electrochemical reactions with controlled flux of precursors, intermediates, and products relies on the team's ability to seamlessly integrate varied catalytic modalities in adaptive cascade reaction architectures. This innovative MURI award has been focused on integrating catalytic cascades from different catalytic modalities such that novel scaffolding and architectures are employed to optimize selectivity, electron transfer, diffusion, and overall cascade flux. The MURI team led by Professor Shelley Minteer from the University of Utah with Professor Scott Banta from Columbia University, Professor Scott Calabrese Barton from Michigan State University, Professor Ian Wheeldon from the University of California Riverside, Plamen Atanassov from the University of New Mexico, and Matthew Sigman from the University of Utah have addressed this research problem through an integrated and collaborative approach. Recently, the team demonstrated the combination of three different classifications of catalysts into a tri-catalytic cascade via redox polymer design.

Last year, the team integrated bioelectrocatalysts with organic oxidation catalysts to extend their utility by enabling significant amplification of the electrocatalytic activity, which increases the rate of electrocatalytic oxidation of glycerol and other alcohols. However, immobilization of organocatalysts is necessary for their use in electrochemical applications. Therefore, the team developed a hybrid tri-catalytic architecture consisting of nanotube catalysts, TEMPO-modified linear poly(ethylenimine) (TEMPO-LPEI), and an enzyme, oxalate decarboxylase (OxDC) (nanotube/TEMPO-LPEI/OxDC) to illustrate a synergistic enhancement in the electrochemical oxidation of glycerol (see FIGURE 6). Specifically, the team demonstrated that immobilized nanotube/TEMPO-LPEI/OxDc permits enhanced electrocatalytic oxidation of glycerol by allowing the organic redox polymer, TEMPO-LPEI, to catalyze the oxidation of glycerol to mesoxalate, followed by cleavage of CO_2 from mesoxalate by catalytically active nanotubes - a crucial step in the complete oxidation of glycerol. Finally, conversion of oxalate to formate by OxDc, and subsequent oxidation of formate by TEMPO-LPEI generates CO_2 while collecting up to 14 electrons per molecule of glycerol. This results in a synergistic enhancement of up to 3.3-fold for this tri-catalytic cascade. This recent accomplishment illustrates the promising potential of surface-immobilized, polymer hydrogel-based hybrid multicatalytic systems, and thus offers a simple methodology for fabricating catalytic cascades.

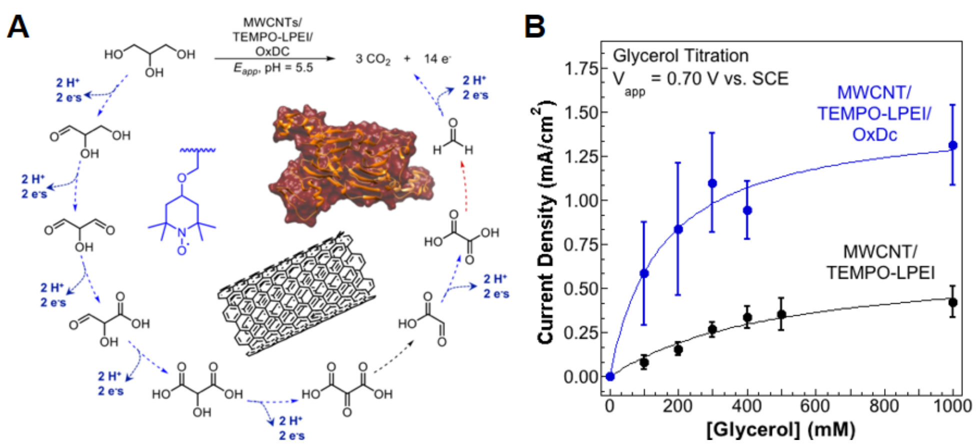

FIGURE 6

Immobilized nanotube/TEMPO-LPEI/OxDc permits enhanced electrocatalytic oxidation of glycerol. (a) Electrocatalytic oxidation cascade of glycerol by MWCNT/TEMPO-LPEI/OxDc multi-catalytic system. Oxidation reactions catalyzed by TEMPO-LPEI are indicated by blue arrows (steps 1 to 5, 7, 9), while decarboxylation reactions catalyzed by MWCNTs and OxDc are shown in black (step 6) and red (step 8) arrows, respectively. (b) Glycerol-induced changes in the catalytic oxidation current by immobilized MWCNT/TEMPO-LPEI (*black curve*) and MWCNT/TEMPO-LPEI/OxDc (*blue curve*). The hybrid multi-catalytic system generates current densities of 0.4 ± 0.1 mA cm^{-2} and 1.3 ± 0.2 mA cm^{-2} for the MWCNT/TEMPO-LPEI and MWCNT/TEMPO-LPEI/OxDc hybrid systems, respectively. Data points fitted into a Michaelis-Menten model.

F. Valence and Dipole-stabilized Resonances in Nitrogen and Silver Fluoride.

Professor Anna Krylov, University of Southern California, Single Investigator Award

Electron attachment to neutral molecules results in formation of anionic species and is a key step in redox and electron-transfer processes. It is also an important process in high-energy environments such as in plasmas, in the presence of strong radiation, and in the detonation region of explosives. The goal of this research is to understand the mechanisms of electron attachment to neutral molecules and the resulting implications.

Depending on the energetics of electron attachment to neutral molecules, resulting anions can be bound or unbound. Unbound ions are transient and decay via autodetachment. These states are metastable, and are sometimes referred to as resonances. Due to their unbound nature, calculation of their physical properties has, until now, been impossible. The researchers have surmounted this problem by use of a complex absorbing potential (CAP) in the wavefunction. This causes the resonance to appear as a state with a normal, finite wavefunction which is integrable, but with a complex energy. A strong advantage of the new method is that it allows the resonance to be treated at the same level of theory as the stationary states.

In FY17, the investigators have applied their CAP method combined with equation-of-motion coupled clusters electronic structure theory to the study of anionic molecular nitrogen and silver fluoride (see FIGURE 7). They found two types of resonances: valence and dipole. The dipole-stabilized resonance was found in silver fluoride and is a new type of resonance which has been discovered by this research (see FIGURE 8).

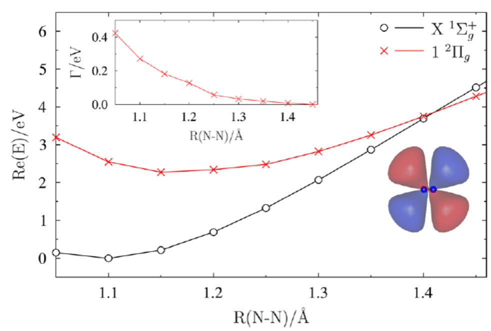

FIGURE 7

Potential energy curves for the 1 $^2\Pi_g$ resonance of N_2^- and the X $^1\Sigma_g^+$ ground state of N_2.

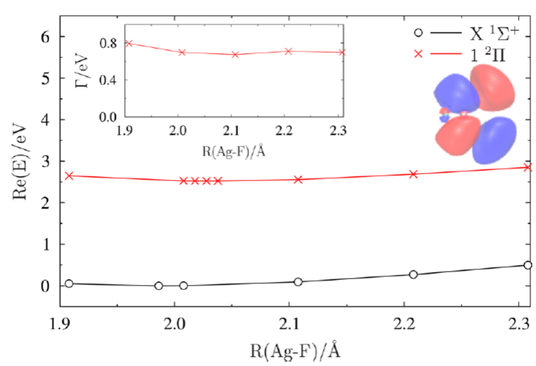

FIGURE 8

Potential energy curves for the 1 $^2\Pi$ resonance of AgF^- and the X $^1\Sigma^+$ ground state of AgF.

The valence shape resonance in N_2^- is stabilized at stretched geometries: the energy of the attached state drops below that of the neutral and its width becomes zero at internuclear distances greater than 1.4 Angstroms. In contrast, energies and lifetimes of dipole-stabilized shape resonances, in which the excess electron resides outside the molecular core, remain nearly constant and do not become bound states by changing the internuclear distance (by vibrational excitation, for example). These results will lead to a better understanding of chemical reactions in high energy environments.

G. Catalytic Reactivity at Nanoscale Metal-Metal Interfaces

Professor Peng Chen, Cornell University, Single Investigator Award

The goal of this research is to decipher the link between interface reactivity and structure/composition in bimetallic nanoparticle catalysts at the single molecule level towards new nanocatalyst design. Previous research used single-molecule super-resolution catalysis imaging in correlation with SEM to directly visualize and quantify the bimetallic activity enhancement on heteronuclear PdAu nanoparticles at the sub-particle level.

In FY17, the research team performed density functional theory (DFT) calculations to gain insight into the mechanism of the experimentally observed enhanced activation of the reactant molecule (resazurin) at bimetallic versus monometallic surface sites (see FIGURE 9). Initially, resazurin interaction with each monometallic surface was studied using Pd(100) and Au(111) as model surfaces. Combining optimized adsorption geometries, crystal orbital Hamiltonian population (COHP) analysis, and the molecular orbitals of resazurin, the researchers were able to schematically depict the forward-donation and back-donation interactions between the metal and the oxygen atom of the resazurin. To computationally evaluate how bimetallic sites could influence the activation of the N-O bond for cleavage, single surface Pd atoms were substituted with Au (Au@Pd) one at a time, and similarly, Au atoms were substituted with Pd (Pd@Au). Calculations indicated that these substitutions resulted in an elongation of the N-O bond by 0.011Å and 0.013 Å, respectively, compared to the monometallic Pd(100) or Au(111) surface sites. The elongation is a result from increases in both forward- and back-donation interactions which ultimately weaken the N-O bond.

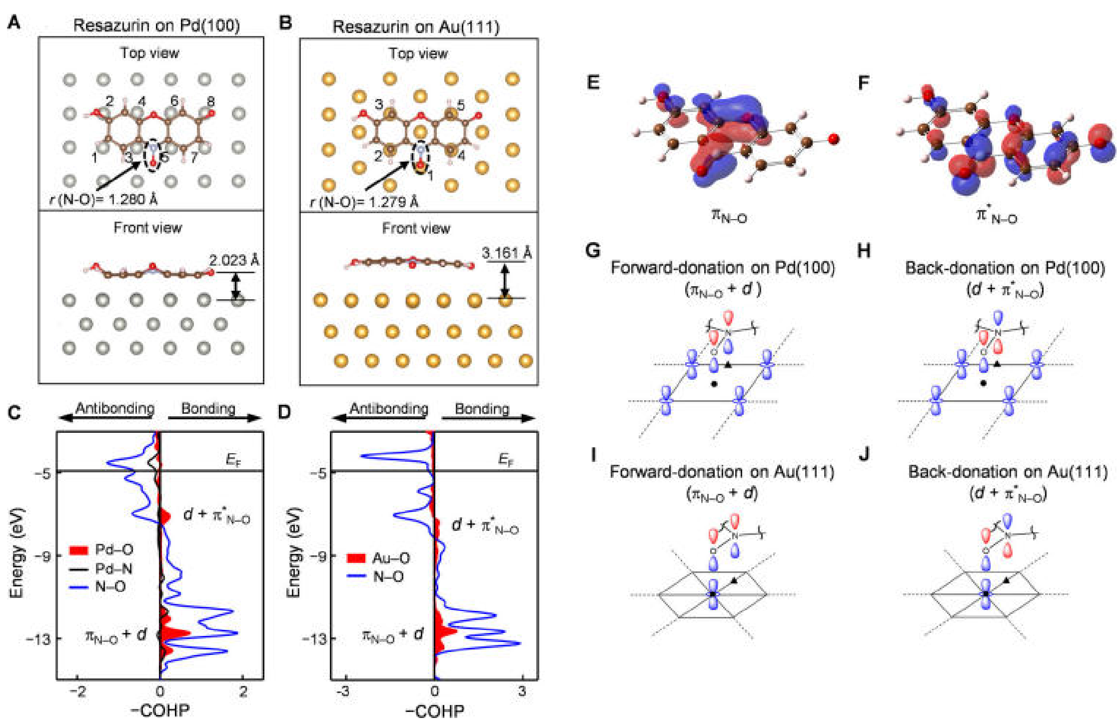

FIGURE 9

Electronic interactions of resazurin with Pd and Au surfaces. (**A**,**B**) Optimized adsorption geometries of resazurin on Pd(100) and Au(111). (**C**,**D**) COHP analyses for the interactions between the N-O fragment of resazurin and the closest metal atoms on Pd(100) and Au(111), respectively. (**E**,**F**) The molecular orbitals of resazurin that are dominantly π_{N-O} (doubly occupied) and π^*_{N-O} (unoccupied) in nature. (**G**,**H**) Schematics of the forward-donation and back-donation on Pd(100). (**I**,**J**) Schematics of the forward-donation and back donation on Au(111).

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Stress-Strengthening Synthetic Polymers by Covalent Mechanochemistry

Investigator: Professor Stephen Craig, Duke University, Single Investigator Award
Recipient: Army Research Laboratory - Weapons and Materials Research Directorate (ARL-WMRD)

The goal of this research is to develop a family of synthetic polymers that undergo activated remodeling via mechanochemistry (ARM) to self-strengthen/self-repair in direct response to mechanical force. One specific aim of this research is to design and synthesize novel cross-linkable, multi-state colorimetric mechanophores (small molecule stress probes) that are capable of reporting their state (inactivated, activated, or cross-linked) through distinct spectroscopic signatures. Through an active research collaboration with ARL-WMRD and the ARL Materials Research Campaign, the researchers are seeking to extend this work to develop colorimetric mechanophores capable of probing not strain rates to potentially serve as early stage damage detection units for high strain rate events such as shock wave propagation associated with traumatic impact. In FY17, the researchers synthesized several spiropyran-based mechanophores and probed their relative activity in elastomers under strain (see FIGURE 10). These materials have transitioned to ARL-WMRD for further characterization.

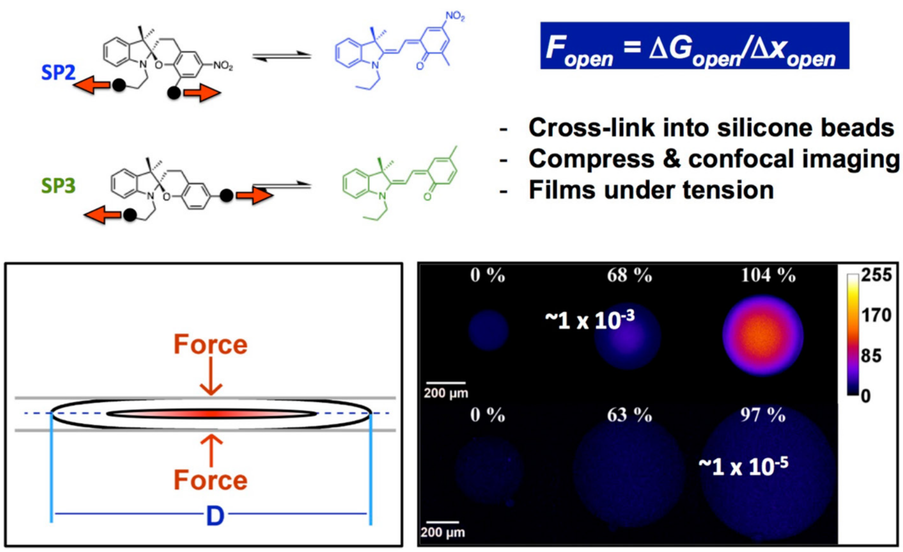

FIGURE 10

Synthesis and characterization of spiropyran-based mechanophores. The activation of different mechanochromic probes occurs at different forces can be quantified by conventional methods. The extent of activation of the probes under deformation can then be quantified in compressed beads by confocal microscopy.

B. Nitrogen Functionalized Carbon Nanostructures from Natural Cotton Fibers and Their Electrocatalytic Properties

Investigator: Professor Guang-Lin Zhao, Southern University and A&M College, Single Investigator Award
Recipient: Argonne National Laboratory

The objective of this research is to develop new and low cost nitrogen functionalized carbon nanostructures as non-precious-metal electrocatalysts for potential energy and related technologies. The team explored a new method for synthesizing carbon nanotubes (CNTs) through catalytic thermolysis of natural cotton fibers, which is a renewable and sustainable agriculture product. Furthermore, the team used pretreated cotton fibers annealing under nitrogen at a temperature of 850°C~1100°C and yield nitrogen-doped CNTs (N-CNTs) with bamboo-like structures. Higher nitrogen doping was obtained by annealing the pretreated cotton fibers in ammonia gas at a similar temperature range. The nitrogen functionalized carbon nanomaterials possess electrocatalytic properties toward oxygen reduction reaction (ORR), when tested by using rotating ring-disk electrode (RRDE) experiments on an electrochemical workstation. The resulting cathodic linear sweep voltammetry (CLSV) data show that the N-CNTs synthesized in ammonia gas environment at a heat treatment temperature of 900°C possessing good ORR activities. These studies transitioned to Argonne National Laboratory for further study to explore potential applications for hydrogen fuel cells and Li-air batteries.

C. Efficient Computational Method for Strong Correlation Effects

Investigator: Professor David Mazziotti, University of Chicago, Single Investigator Award
Recipients: RDMChem, LLC and ARL-WMRD

The goal of this research was to develop fundamental physical theories to describe the electronic structure of a many-electron system with only two electrons by replacing the wave function by the two-electron reduced density matrix (2-RDM) as the basic variable for quantum many-electron theory. Professor Mazziotti has been successful in developing all of the fundamental physical theories needed to achieve a 2-RDM representation of a muli-electron system. The results of his work have transitioned to RDMCHEM, LLC.

RDMCHEM is developing the next generation of computational software for chemistry with applications to problems in chemistry, engineering, molecular biology, and physics. The software will enable unprecedented quantitative predictions on highly correlated molecules and materials, especially excited states, open systems, and time-dependent systems. Current computational software designed for describing strong correlation scales exponentially in computer runtime with system size. The new software achieves a low polynomial computational scaling with applications to molecular systems of unprecedented size (see FIGURE 11). The software will lead to opportunities for the design of strongly correlated materials for energy capture, storage, and transfer as well as for tunable thermal and thermo-electric properties, the prediction of spectroscopic signatures of chemical agents, and the processing and analysis of noisy visual, audio, or electromagnetic data for advanced sensing. Both the chemistry software and the mathematical optimization software "under the hood" are being commercialized for a wide customer base spanning the government, industrial, and academic research centers. A beta version of RDMChem transitioned to scientists at ARL-WMRD in FY17 for testing.

Features	RDMChem	Gaussian	Schrödinger	Molpro	Q-Chem
Price	LOW	HIGH	HIGH	HIGH	HIGH
Can Treat Large Strongly Correlated Molecules?	YES	NO	NO	NO	NO
Has Proprietary 2-RDM Compression for DFT-like scaling?	YES	NO	NO	NO	NO
Multi-core Parallelization in Base Price?	YES	NO	YES	NO	NO
Molecular Visualization Included?	YES	NO	NO	YES	YES
Has Interfaces with Maple, Mathematica, and/or MATLAB?	YES	NO	NO	NO	NO
Has HS/College Classroom License?	YES	NO	NO	NO	NO

FIGURE 11

Comparison of RDMChem software features to state-of-the-art commercially available software.
RDMChem has significant advantages in both price and quality features in comparison to commercially available alternatives.

D. Determination of Oxygen and Hydrogen Mass Transfer Coefficients in PEMFC GDE and Separation into Gas and Electrolyte Contributions
Investigators: Professors T.V. Reshetenko and J. St-Pierre, University of Hawaii, Single Investigator Award
Recipients: Nuvera Inc, 3M

The objective of this research is to develop and validate a method of determination of reactant mass transfer coefficients in proton exchange membrane fuel cells (PEMFCs). The method is based on measurements of the limiting current distribution and utilizes operation at a low reagent concentration (O_2 or H_2) and dilution with different inert gases (from He to C_3H_8) which allows researchers to separate the gas phase molecular diffusion coefficient and a combination of diffusion in fine pores (Knudsen diffusion) and ionomer/water films.

In FY17, the effects of the gas diffusion layer (GDL) structure, in particular loading of microporous layer (MPL), on the oxygen mass transfer coefficient were studied. An increase in the microporous layer loading from 0 to 150 % of the baseline value not only slowed diffusion through fine pores and ionomer/water films but also affected gas phase molecular diffusion and the total fuel cell performance. Data demonstrated that an optimal MPL loading exists, which correlates with textural GDL properties and provides desirable mass transfer properties and fuel cell performance. The methodology was applied to Nuvera's single cell open flow field (SCOF) design. It was shown that the separation method is applicable to industrially relevant flow field designs thus extending its usefulness beyond the original focus on serpentine flow fields. Analyses completed with the limiting current model and an electrochemical impedance model for cross-validation showed that these two methods provided comparable values of the oxygen mass transfer coefficient. The impacts of variations in operating conditions (temperature and gases humidification) on O_2 mass transfer coefficients for Nuvera's SCOF design were also evaluated. Results revealed a decrease in the rate of diffusion through fine pores and ionomer/water films for saturated gas streams which showed complex interactions between water flooding, ionomer permeability and gas transport in fine pores. These results have transitioned to Nuvera Inc. and 3M for further validation and use of the methodology to improve the understanding of transport issues in PEMFCs. These activities are expected to address the DoD need for smaller power units.

E. Molecule-Surface Dynamics in Functionalized Mesoporous Silicon
Investigator: Professor Sharon Weiss, Vanderbilt University, Single Investigator Award
Recipient: ARL-SEDD

The objective of this research, led by Professor Weiss, was to investigate the impact of surface chemistry and morphology on the surface interaction mechanisms involved in diffusion and molecular attachment of chemical and biomolecular species in nanoporous materials. Computational and experimental studies compared analyte transport and reaction in closed- versus open-ended porous silicon films. Studies with molecules with varied molecular weight and diffusivities in porous silicon films with fixed pore morphology (25 nm, average pore diameter) and functionalization suggest that significantly improved response times can be achieved when a flow-through scheme is employed that facilitates more efficient mass transport of a large analyte (>1kDa) with slow diffusivity ($D<10^3$ $\mu m^2/s$) in the pores.

In FY17, this research transitioned to ARL-SEDD through a cooperative agreement established with Vanderbilt University to jointly explore functionalization Professor Weiss' porous silicon films with ARL's peptide-based capture agents. Initially, the PI will investigate nanostructured porous silicon and flat silicon substrates, and carry out experiments to gain an understanding of diffusion and attachment dynamics. The flow-through porous silicon membranes can be fabricated in a microarray platform that is well-suited to carry out label-free detection of multiple analytes in a single parallel experiment and, at the same time, evaluate the efficacy of peptide-based capture agents on a solid sensor surface in a high-throughput approach. Professor Weiss' nanostructured porous silicon substrates offer a unique platform designed to act as a transducer for optical biosensing.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Sequence Defined Polymers

Professor Christopher Alabi, Cornell University, Single Investigator Award

The objective of this project is to create a new class of sequence-defined and architecturally diverse polymers that can be used to investigate the relationships between primary sequence and intrinsic macromolecular properties such as secondary structure, folding and self-assembly. The long-term goal is to use precise polymers to program the assembly of functional macromolecular architectures and materials with unique properties, which requires an understanding of the behavior and dynamics of these polymers. In FY17, research efforts focused on investigating the contributions of synthetic length, pendant group charge, and backbone hydrophobicity to the structure and dynamics of sequence-defined oligothioetheramides (oligoTEAs; see FIGURE 12).

It is anticipated that in FY18, the researchers will refine the synthetic strategy used for the assembly of these oligoTEAs such that they can be created at scale without a support. Furthermore, the team will explore the precise-sequence control of the oligoTEA backbone to tune the bulk properties of cross-linked polymer networks, focusing on using sequence to modulate the mechanical response and reprocessability of the resulting polymer network. If successful, these studies may lead to the first programmable synthetic sequence-defined hierarchical assembly modalities that could find use in a variety of applications and materials of interest to Army.

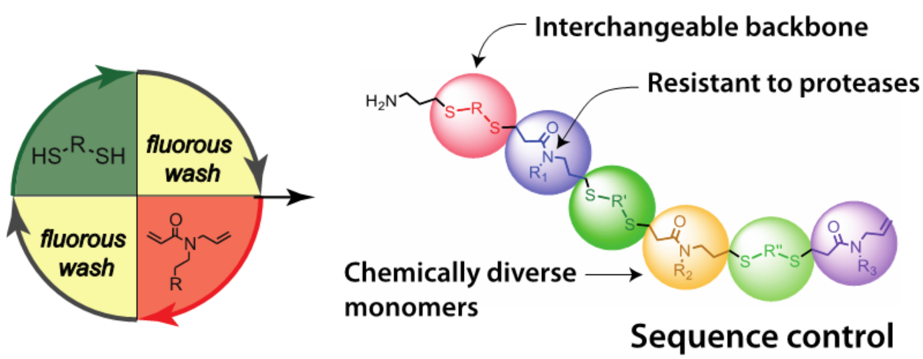

FIGURE 12

Synthesis of sequence-defined oligothioetheramides (oligoTEAs).

B. Non-Thermal Chemical Reactions at Metal Nanostructure Surfaces

Investigator: Professor P. Christopher, University of California - Santa Barbara, Single Investigator Award

The general goal of this project is to utilize a comprehensive and combined experimental-computational approach to develop mechanistic descriptions of catalysis by metal nanostructures when excited via a non-thermal energy sources such as photons, electrons, and ions. The overall objective is to mechanistically characterize the most efficient and bond-selective selective approaches for driving chemical conversion processes at metal nanoparticle surfaces through non-thermal excitation mechanisms. In FY18, it is anticipated that the research team will explore the chemistry mediated by Ag and Pt surfaces associated with CO and NO desorption and dissociation as driven by photons or electrons independently, or through non-thermal plasma excitation with varied sample bias (to control the flux of impinging charged species). When coupled with theoretical calculations, this will begin to provide insights into the most efficient and bond selective approaches for driving surface chemistry through non-thermal excitation.

C. Supported Single Atom Catalysts for Low Temperature Oxidation
Professor Ayman Karim, Virginia Tech, Single Investigator Award

The objective of this research is to decouple the effects of the metal nuclearity and electronic properties of supported single atom catalysts on the catalytic activity for low temperature oxidation. Initial research in FY17 focused on the synthesis, characterization, and preliminary catalytic studies of different size Ir-supported catalysts. Three catalysts were selected for these studies (see FIGURE 13). The oxidation kinetics for CO were measured, revealing that the CO and O_2 reaction orders were -1 and +1 on the large nanoparticles; however, as the IR size decreased towards subnanometer clusters and single atoms, the CO order increased and became positive and the O_2 order decreased to approximately zero (see FIGURE 14). The orders suggest the reaction mechanism is very different on the subnanometer clusters and single atoms compared with the mechanism on large nanoparticles where the metal sites are poisoned by CO. *In situ* infrared spectroscopy results with the 0.05% catalyst suggest that O_2 adsorption becomes competitive with CO on small clusters and single atoms which is consistent with the change in reaction orders as the Ir size decreases. Density functional theory calculations of Ir single atoms supported on $MgAl_2O_4$ are also consistent with positive order in CO and approximately 0 order in O_2.

It is anticipated that in FY18, the team will explore the synthesis mechanisms to achieve 100% single atoms with higher loadings and 100% subnanometer clusters on $MgAl_2O_4$ and $ZnAl_2O_4$, and study their activity for CO oxidation. This effort will provide a fundamental understanding of catalyst structure:activity relationships in the subnanometer regime and impact Army relevant areas in novel catalyst designs for decontamination.

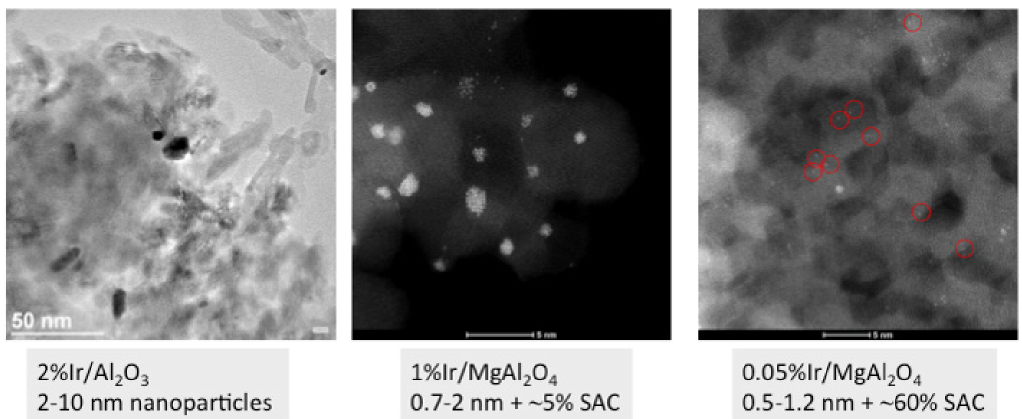

FIGURE 13

Micrographs of catalysts used in oxidation studies. Transmission electron microscopy and aberration-corrected scanning transmission electron microscopy images of (from left to right) 2%Ir/Al_2O_3, 1% $Ir/MgAl_2O_4$ and 0.05% $Ir/MgAl_2O_4$. Single atoms are highlighted with red circles.

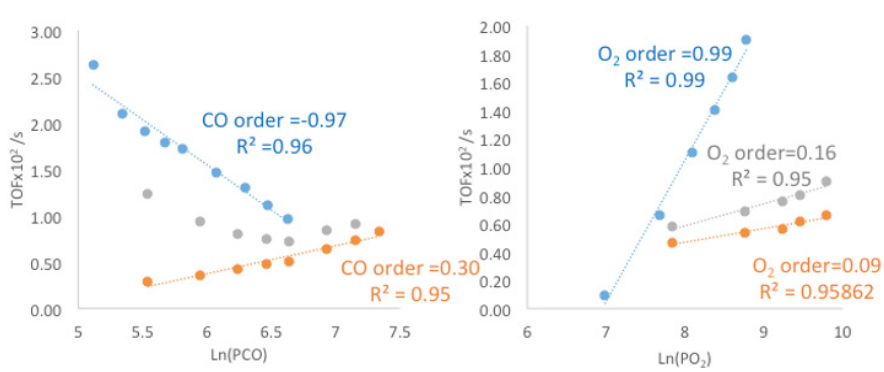

FIGURE 14

CO oxidation kinetics. Reaction conditions: T = 155°C; for CO order (left), 10kPa O_2, 0.1-0.7 kPa CO; for O_2 order (right), 1 kPa CO, 1-14 kPa O_2.

D. Ultrafast Dissociation Dynamics in the Radical Cations of Nitrotoluenes
Professor Katharine Tibbetts, Virginia Commonwealth University, STIR Award

The objective of this research is to apply femtosecond pump-probe techniques for studying initial dissociation dynamics in the radical cations of nitrotoluenes, which are important model systems for nitroaromatic energetic materials. To prepare the radical cations in the ground electronic state, the PI will use the recently developed method of adiabatic ionization with strong field near-infrared femtosecond laser pulses. The subsequent dissociation dynamics will be probed with weak field pulses at varying wavelengths to access the cationic excited states. Through complementary theoretical calculations of the ionic ground and excited state potential energy surfaces (PES's), the PI will investigate the roles of electronic excitation and nonadiabatic relaxation through conical intersections in initiating bond cleavage events.

In FY18, it is anticipated that the PI will selectively access the ionic excited state leading to NO2 loss in each of three different nitrotoluene isomers. The optimal probe wavelength to maximize population transfer in each molecule will be determined and compared with their corresponding energies to the calculated excited state energies. Collectively, these studies will enable validation of the calculated excited state energies in each molecule and determination of the relative excited state energies of each isomer. Furthermore, the demonstration of selective production of distinct dissociation products when using different probe wavelengths and pump-probe delay times would represent a promising initial step towards selective initiation of detonation processes in energetic molecules using laser excitation. Determining the energies of PES's, locations of conical intersections, and relaxation timescales driving particular dissociation pathways may enable optical control over the decomposition processes through selective bond cleavage. This capability would be advantageous for designing energetic molecules amenable to detonation by photoinitiation, which has been a longstanding goal in energetic molecule research.

E. Oxygen and Hydrogen Mass Transfer Coefficients in Proton Exchange Membrane Fuel Cells
Professor T.V. Reshetenko, University of Hawaii, Single Investigator Award

The objective of the research is to develop and validate a novel method of determination and subsequent deconvolution of reactant mass transfer coefficients in proton exchange membrane fuel cells (PEMFCs) gas diffusion electrodes (GDEs). The proposed study will reveal fundamental aspects of oxygen and hydrogen transport in GDEs as well as critical factors affecting diffusion processes in multiphase, porous and confined environments. It is anticipated that in FY18, the team will determine the effects of pressure and gas humidification on oxygen mass transfer coefficients, because these operating parameters respectively impact the gas phase molecular and Knudsen diffusion as well as transport in the ionomer (the size of hydrophilic channels responsible for gas transport is dependent on ionomer water content). A study of the effects of ionomer loading on the oxygen mass transfer coefficients is also planned to clarify differences between nano-structured thin film technology (3M) and more traditional electrode layer designs. Finally, investigations will be expanded to the characterization of hydrogen mass transport processes of relevance to recirculation systems and fuel gas streams diluted by nitrogen crossing over from the cathode compartment.

VI. DIVISION AND DIRECTORATE STAFF

A. Division Staff

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Program Manager (Acting), Reactive Chemical Systems

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Program Manager, Electrochemistry

Dr. James Parker
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Dr. Laura Krnavek
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Dr. Peter Reynolds
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Dr. Kelby Kizer
Physical Scientist and Technical Assistant to the PSD Director

Mr. John McConville
Technology Transfer Officer, Institute for Soldier Nanotechnologies

Ms. Ivory Chaney
Administrative Specialist

Ms. Wanda Lawrence
Contract Support

CHAPTER 4: COMPUTING SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2017* is to provide an annual historical record summarizing the programs and basic research supported by ARO in FY17. ARO's mission is to support creative basic research resulting in new science that enables new materials, devices, processes, and capabilities for the current and future Soldier. This chapter provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions enabled by the ARO Computing Sciences Division in FY17.

A. Scientific Objectives

1. Fundamental Research Goals. The principal objective of the ARO Computing Sciences Division is to build the fundamental principles and techniques governing computational methods, models, and architectures to establish the foundation for revolutionary advances in intelligent, trusted, and resilient computing that provide increased performance and computational capability to enhance warfighter situational awareness, decision making, command and control, and weapons systems performance. The Division supports basic research in new computing architectures and models for intelligent and trusted computing in data fusion and extraction techniques for efficient information processing, to create new capabilities in social informatics, and in resilient computing systems for mission assurance. The results of these efforts will stimulate future studies and help keep the U.S. at the forefront of computing sciences research.

2. Potential Applications. This program identifies and addresses the Army's critical basic research problems in the computing sciences where progress has been inhibited by a lack of novel concepts or fundamental knowledge. Computing science is pervasive in nearly all Army systems, particularly Command, Control, Communications, Computing, Intelligence, Surveillance, and Reconnaissance (C4ISR) systems. The number of information sources on the battlefield will grow rapidly; computing and information science research must provide capabilities to process this in real-time and ensure that Soldiers and commanders do not experience information overload that could adversely affect their ability to make decisions. Also, in spite of the increased complexity of future battlefield information systems, dependence on them will only increase, therefore they must be extremely reliable and secure. Research in this program has application to a wide variety of developmental efforts and contributes to the solution of technology-related problems throughout the Army's Future operational goals. For this reason, computing science is a key technology underpinning future Army operations.

3. Coordination with Other Divisions and Agencies. The Computing Sciences Division supports ARL's Information Sciences Campaign in the areas of information understanding, information fusion, and computational intelligence. Collaborative efforts aim at discovering scientific principles and creating innovative frameworks and analytical approaches for the representation, dimensionality reduction, information content extraction, and integration of multimodal data that will revolutionize information processing to convert data into actionable intelligence to support Army information processing. A joint workshop was organized by the division and the ARL Cyber Security Research Consortium to explore new research opportunities in moving target cyber defense. The Computing Sciences Division has worked with ARL's Computational and Information Sciences Directorate (CISD) to develop two new Small Business Technology Transfer (STTR) projects that will enhance computational capability through novel computing system architectural design. Division staff have engaged the ARL Human Sciences Campaign and the Sciences-for-Lethality and Protection Campaign to create a new computer simulation capability for acoustic modeling for human studies and for radio frequency (RF) propagation in urban environments. The Division's research portfolio also supports the ARL ERAs of (i) Intelligent Teams, (ii) Impact of Operating in a Contested Environment, and (iii) Implementation.

The Division's research investment strategy is coordinated with partner disciplines and computer scientists at ARO, other directorates within ARL, other Army agencies, and related programs in other DoD and Federal organizations. The Division's research portfolio is supported by Army basic research Core funding with substantial additional resources from the Assistant Secretary of Defense for Research and Engineering [ASD(R&E)], including the Multidisciplinary University Research Initiative Program (MURI), and from other agencies, such as the Defense Advanced Research Projects Agency (DARPA).

To effectively meet Division objectives and to maximize the impact of potential discoveries for the Army and the nation, the Computing Sciences Division frequently coordinates and leverages efforts with Army scientists and engineers and with researchers in other DoD agencies. In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the ARO Life Sciences Division include promoting research to investigate effective human-computer communication mechanisms and developing new metrics and benchmarks for social media analysis. The Division also coordinates efforts with the Network Sciences Division to explore new techniques for robust and resilient mobile ad hoc networks, to establish adversarial models for effective cyber defense, and to investigate fundamental principles for trusted social computing. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas. Each of the Program Areas within the Division balances opportunity-driven research with high risk, high-payoff scientific exploration and needs-driven efforts that look for scientific solutions to the near-term needs of the warfighter.

B. Program Areas

The Computing Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY17, the Division managed research within these five Program Areas: (i) Information Processing and Fusion, (ii) Computational Architectures and Visualization, (iii) Information and Software Assurance, (iv) Intelligent Systems, and an International Program, (v) Advanced Computing. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Information Processing and Fusion. The goal of this Program Area is to understand the fundamental principles and to establish innovative theories for data processing, information extraction, and information integration toward real-time situational awareness and advanced targeting. There are three thrusts for this program area: (i) foundations of image and multimodal data analysis, (ii) data and information fusion, and (iii) active and collaborative sensing. With the ubiquitous availability of data acquisition capabilities in future military operations, effective data and information processing is of increasingly critical importance to defense missions. This program emphasizes mathematical theories, methodologies and algorithms for image understanding, video analysis, and data/information fusion. This research supports the development of novel representations of multimodal data to enable the understanding of multimodal sensor data and contextual information. Also supported is research on detection of events, actions, and activities to extract activity-based intelligence, especially when the events are rare and no extensive training data is available. Potential applications include detection of improvised explosive devices and persistent surveillance.

The increased capability of electronic systems and the proliferation of sensors are generating rapidly increasing quantities of data and information to the point that system operators and commanders are overwhelmed with data and saturated with information. An area of increasing importance is data and information integration or fusion, especially fusion of data from disparate sensors and contextual information. Research activities address several basic issues of data fusion, including information content characterization of sensor data, performance modeling, and the value of information.

2. Computational Architectures and Visualization. The two main Thrusts of this Program Area are Computational Architectures (CA) and Visualization (V). The goal of the CA Thrust is to discover new effective architectures, computational methods, and software tools for future computing systems with special emphasis on the effect that the technological shift to heterogeneous, multi-core processors will have on newly-developed systems. The goal of the V Thrust is to make very large simulations and the visualization of massive data sets more computationally efficient and more interactive for the user. An overarching theme for both Thrusts is the efficient managing and processing of massive data sets. This is due to the fact that the Army's ability to generate data of all types from the battlefield to the laboratory far outpaces the Army's ability to efficiently manage, process, and visualize such massive amounts of information. The CA Thrust attempts to address this issue by investigating innovative architectural designs of both hardware and software components and their interfaces. The V Thrust addresses the issue by investigating innovative algorithms to render massive data sets and/or massive geometric models and to perform large scale simulations of importance to the Army.

The long-term payoffs of the CA Thrust for the Army include new computer modeling and design concepts (or paradigms) as well as software libraries that take advantage of these new multi-core processors and that are scalable (usable on large-scale complex problems and able to handle massive amounts of data) and accurate (precise enough to predict and detect phenomena of interest) for both the laboratory and the battlefield. A payoff associated with the V Thrust is the development of more efficient, interactive, and physically realistic battlefield, training, and scientific simulations.

3. Information and Software Assurance. The goal of this Program Area is to understand the fundamental principles of robust and resilient cyber information systems that can enable the corresponding functions to be sustained under adversarial conditions. The studies guided by this program will enable and lead to the design and establishment of trustworthy computing and communication, regardless of threat conditions. The ARO program on Information Assurance currently has two major Thrust areas: (i) Highly Assured Tactical Information and (ii) Resilient and Robust Information Infrastructure. The goal of the Highly Assured Tactical Information Thrust is to gain new scientific understandings for trustworthy tactical communications and for establishing fundamental principles and to ensure their trustworthiness. The Resilient and Robust Information Infrastructure Thrust promotes research on cyber situation awareness theories and frameworks that combines intrusion prevention, detection, response, and recovery to establish fundamental scientific principles for building mission-sustaining information systems (e.g., software/hardware, computing/communication systems).

Within these research areas, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goal. Research in the Resilient and Robust Information Infrastructure Thrust is focused on exploring and establishing resilient computing and survivability principles, and understanding system trade-offs such as performance, resiliency, and, survivability. The Highly Assured Tactical Information Thrust may lead to the development of novel situation awareness theories and techniques that help defenders obtain an accurate view of the available cyber-assets, to automatically assess the damage of attacks, possible next moves, and impact on cyber missions, and to model the behavior of adversaries to predict the threat of future attacks on the success of a mission. The warfighters must have unprecedented situational awareness (including enemy and friendly awareness) at all times. Information assurance must address the delivery of authentic, accurate, secure, reliable, timely information, regardless of threat conditions, over heterogeneous networks consisting of both tactical (mobile, wireless) and fixed (wired) communication infrastructures.

4. Intelligent Systems. The goal of this Program Area is to establish the scientific foundation of next generation intelligent systems and create cutting-edge capabilities in machine learning that can greatly enhance the Army's capabilities in mobility, agility, lethality, and survivability. There are two main research thrust areas: (i) Advanced Learning and (ii) Intelligent Systems.

The Advanced Learning thrust focuses on establishing the theoretical foundation of machine learning. New learning approaches will need to be addressed for both dimensionality challenges and temporal characterization of "big data," which may evolve continuously. In addition, new techniques must address robustness where the learning system will be able to deal with incorrect input due to noise and observation errors, and potentially malicious input that aims to disrupt learning. Adaptation in learning is another major challenge. It is conceivable that due to complexity, non-steady behaviors, fast changing context and environment, it may not ever be possible to fully capture a dynamic changing world, especially under the condition of incomplete information and with information uncertainties. It is critical to develop an advanced system that can continuously learn, update its knowledge base accordingly, and dynamically adapt its reasoning, decisions, and actions.

The Intelligent Systems thrust focuses on creating autonomous entities with advanced cognitive capabilities that can successfully integrate advanced learning, knowledge representation and organization, cognitive reasoning, adaptation, and autonomous action. Quite often intelligence systems are engaged in sensing, perception, reasoning and understanding, learning, collaboration, and take actions in an autonomous way. For these systems, sensing and vision processing play a critical role in learning, perception, and establish situation awareness for decision making and for intelligent actions such as navigation, while language processing and communication help build coordination, collaboration, and contribute to a shared knowledge base, planning, and team decision making. A common trait of intelligent systems lies in their capability to process information along with suitable context and environment to make the best decisions and to take appropriate actions. An ideal intelligence system should have a strong cognitive capability that enables itself to deal with environmental changes, to carry out new tasks, and to cope with unknown situations.

5. Advanced Computing (International Program). The goal of this program area is to develop novel computing capabilities, both at the hardware and software levels, that support future army data analysis needs with enhanced security and situational awareness built in from design. Such capabilities must meet the task specific footprint requirements for the mission. The program is pursuing four main thrusts: (i) large data science and analytics, (ii) next-gen computing architectures and algorithms, (iii) task specific computing architectures, networks, and algorithms, and (iv) security and algorithms for future cyber infrastructure. Large data science and analytics is pursuing holistic data analysis approaches to deal with the “Big Data” problem from collection through analysis to interpretation. Next-gen computing architectures and algorithms is seeking novel approaches to hardware compute platforms that may be derived from novel approaches to algorithms or independently modeled; as neuromorphic computing is modeled off of human brain synapses. Task specific computing architectures, networks, and algorithms desires research into compute and algorithm platform designed to meet footprint requirements for specific missions, optimizing for a subset of size, weight, energy, temperature, performance, and security. Security and algorithms for future cyber infrastructure focuses on novel cyber security solutions from the ground up such as next generation cyber infrastructures and the security of modern platforms, such as IOT (Internet of Things) devices.

The growing reliance on compute capabilities, communication, and data analysis for mission success require significant advances in computing and algorithmic capabilities to meet the ever growing challenges of data scale, hostile environments, and user requirements. The payoff of this program area will be new capabilities to provide soldiers in the field with the compute capabilities to provide more advanced analysis capabilities with reduced weight, longer mission sustainability, and more rapid response; all with reduced susceptibility to hostile environments.

C. Research Investment

The total funds managed by the ARO Computing Science Division for FY17 were $53.3 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY17 ARO Core (BH57) program funding allotment for this Division was $6.7 million and $0.8 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $4.6 million to projects managed by the Division. The Division also managed $8.7 million of Defense Advanced Research Projects Agency (DARPA) programs, and $3.4 million provided by other Federal agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $0.9 million for contracts. The Institute for Creative Technologies received $26.3 million. In addition, $1.9 million was provided for awards in the Historically Black Colleges and Universities and Minority Serving Institutions (HBCU/MSI) Programs, including funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY17 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY17 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY17, the Division awarded 25 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Ehab Al-Shaer, University of North Carolina - Charlotte; *Multi-layer Resilient Active Cyber Defense - Metrics, Synthesis, Evaluation, and Verification*
- Professor James Anderson, University of North Carolina - Chapel Hill; *Mixed-Criticality Real-Time Computing with GPUs*
- Professor Reza Azarderakhsh, Florida Atlantic University; *Emerging side-channel resistant and resource-friendly elliptic curve algorithms and architectures*
- Professor Waheed Bajwa, Rutgers, The State University of New Jersey - New Brunswick; *Robust, Decentralized Feature Learning from Big Data*
- Professor Feng Chen, State University of New York (SUNY) at Albany; *Uncertainty Management for Dynamic Decision Making*
- Professor Yingying Chen, Stevens Institute of Technology; *Enhanced Learning of Sensor Fusion for Human Authentication*
- Professor Yun Fu, Northeastern University; *Images Assisted Video Recognition by Heterogeneous Knowledge Transfer*
- Professor Somesh Jha, University of Wisconsin - Madison; *Robustness and Stability for Data Analysis in Security*
- Professor Yier Jin, University of Florida - Gainesville; *Bridging the Hardware-Software Gap: A Proof-Carrying Approach for Computer Systems Trust Evaluation*
- Professor Marcelo Kallmann, University of California - Merced; *Algorithms for Visualization and Simulation of Optimal Navigation*
- Professor Murat Kantarcioglu, University of Texas at Dallas; *Data Analytics for Cyber Security: Defeating the Active Adversaries*
- Professor Ramesh Karri, New York University; *Secure DNA Forensics Using Microfluidic Biochips*
- Professor Sneha Kasera, University of Utah; *Preventing Radio Window Attacks*

- Professor James Keller, University of Missouri - Columbia; *Multiple and Multi Sensor Research for Explosive Hazard Detection*
- Professor Lu Long, Research Foundation of SUNY at Stony Brook University; *Enabling Secure Integration of Web and Mobile: A Principled Multi-level Approach*
- Professor Partha Pande, Washington State University; *Energy Efficient Heterogeneous Datacenter-on-Chip for Big Data Computing*
- Professor Balakrishnan Prabhakaran, University of Texas - Dallas; *Robustness Studies in 3D Camera Data*
- Professor Ana Ramirez, Universidad Industrial de Santander; *Full Waveform Inversion for Ground Penetrating Radar*
- Professor Ribeiro Alejandro, University of Pennsylvania; *Geometric and Graph Structures in Information Characterization and Extraction*
- Professor Jie Shan, Purdue University; *Scene Modeling through Multi-modal Geospatial Data Fusion*
- Professor Pavan Turaga, Arizona State University; *Scalable topological and geometric methods for multimodal activity modeling*
- Professor Joseph Wilson, University of Florida - Gainesville; *Algorithm and Decision Support for Vehicle Mounted Mine Detection Systems*
- Professor Shouhuai Xu, University of Texas at San Antonio; *MTD Dynamics: A Quantitative Framework for Modeling and Orchestrating Moving-Target Defense*
- Professor Chuan Yue, Colorado School of Mines; *Enabling and Securing Robotic Team Situational Awareness*
- Professor Alina Zare, University of Florida - Gainesville; *Multi-Sensor Fusion for Buried Object Detection*

2. Short Term Innovative Research (STIR) Program. In FY17, the Division awarded two new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Rafail Ostrovsky, University of California - Los Angeles; *Towards Provably Secure Malware Defenses*
- Professor Jie Wu, Temple University; *Moving Target Defense in Military Organization with Connected Dominating Set as Command Units*

3. Young Investigator Program (YIP). In FY17, the Division awarded four new YIP projects to drive fundamental research in an area relevant to the current and future Army. The following PIs and corresponding organization were a recipient of the new-start YIP award.

- Professor Yong Jae Lee, University of California - Davis; *Foundations of Image and Multimodal Data Analysis*
- Professor Marvin Onabajo, Northeastern University; *An On-Chip Thermal Sensing Method to Detect Malicious Integrated Circuits*
- Professor Dong Wang, University of Notre Dame; *Reliable Multimodal Data Fusion from Physical and Human Sensors with Quality Assurance*
- Professor Meng Wang, Rensselaer Polytechnic Institute; *Feature Extraction from Large-Scale Complex and Imperfect Data*

4. Conferences, Workshops, and Symposia Support Program. The Division provided funds in support of a range of scientific conferences, workshops, and symposia that were held in FY17. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences, with the goal of supporting scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army, and to define the research needs, thrusts, opportunities, and innovation crucial to the future Army. Proposals requesting funding support, typically for less than $10K, were received and evaluated in line with the publicly available ARO BAA. In FY17, four proposals were selected for funding by the Division in FY17 to support conferences, workshops, or symposia.

5. Special Programs. In FY17, the Division also awarded five new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school and undergraduate students. These efforts were funded through the ARO Core Program and Youth Sciences Programs, for research to be performed at academic laboratories currently supported through active SI awards (refer to CHAPTER 2, Section IX).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Computing Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Adversarial and Uncertain Reasoning for Adaptive Cyber Defense: Building the Scientific Foundation. This MURI began in FY13 and was awarded to a team led by Professor Sushil Jajodia of George Mason University. Adaptive defense mechanisms are essential to protect our nation's critical infrastructure (computing, communication, and control) from sophisticated adversaries who may stealthily observe defense systems and dynamically adapt their attack strategies. This research aims to create a unified scientific foundation to enable the design of adaptive defense mechanisms that will maximize the protection of cyber infrastructure while minimizing the capabilities of adversaries.

The research will leverage recent advances in security modeling, network science, game theory, control theory, software system and network protocol security to create the scientific foundation, which may include general models for defense mechanisms and the systems they protect as well as irrational and rational adversaries. This research will develop a new class of technologies called Adaptive Cyber Defense (ACD) that will force adversaries to continually re-assess, re-engineer and re-launch their cyber attacks. ACD presents adversaries with optimized dynamically-changing attack surfaces and system configurations, thereby significantly increasing the attacker's workloads and decreasing their probabilities of success.

2. Noncommutativity in Interdependent Multimodal Data Analysis. This MURI began in FY16 and was awarded to a team led by Professor Negar Kiyavash at the University of Illinois at Urbana-Champaign. The goal of this research is to establish a new comprehensive information theory for data analysis in noncommutative information structures intrinsic to hierarchical representations, distributed sensing, and adaptive online processing. Methods will be developed based on a novel theory in conjunction with the latest theories of information, random matrices, free probability, optimal transport, and statistical machine learning. They will be applied to the technical domains of causal inference, adaptive learning, computer vision, and heterogeneous sensor networks, and will be validated on real-data test beds including: (i) human action and collective behavior recognition, and (ii) crowd-sourcing in a network of brain-machine interfaces. The framework will provide answers to questions such as: What are the fundamental performance limits for noncommutative information collection and processing systems? What is the effect of side information on noncommutative information structures? How can low complexity proxies for performance be defined that approximate or bound noncommutative performance limits? How can noncommutativity of adaptive measurements be exploited to improve fusion, processing, and planning for distributed sensing systems? When do sequential or partially ordered designs offer significant performance gains relative to randomized designs like compressive sensing?

The approaches for extracting knowledge from complex irreversible partially ordered information structures include but are not limited to introduction of information divergence measures over noncommutative algebras, noncommutative relative entropy measures, and estimation techniques for such measures for high-dimensional data. Accounting for noncommutative structures will result in fundamentally new ways of fusing ordered, directed, or hierarchical organized information to support timely decisions at the appropriate level of granularity. Humans learn actively and adaptively, and their judgments about the likelihood of events and dependencies among variables are strongly influenced by the perception of cause and effect, whereas man-made systems only employ correlation-type symmetric measures of dependencies. Research will lead to the development of a theory of decentralized information sharing, causal inference, and active learning inspired by human decision making. Establishment of such a theory for sensing and data processing and application of it to grand challenges in computer vision and brain-computer interfaces will provide new capabilities, including improved time-sensitive, dynamic, multi-source information processing, actuation, and performance prediction guarantees.

3. Closed-Loop Multisensory Brain-Computer Interface for Enhanced Decision Accuracy. This MURI began in FY16 and was awarded to a team led by Professor Maryam Shanechi at the University of Southern California. The goal of this research is to create new methodologies for modeling multimodal neural activity underlying multisensory processing and decision making, and to use those methodologies to design closed-loop adaptive algorithms for optimized exploitation of multisensory data for brain-computer communication.

This research effort will contribute to the development of a new closed-loop brain-computer interface (BCI) framework for enhancing decision accuracy. The framework will collect multimodal neural, physiological, and behavioral data, decode mental states such as attention orientation and situational awareness, and use the decoded states as feedback to adaptively change the multisensory cues provided to the subject, thus closing the loop. To realize such a framework, the effort will make fundamental advances on four fronts, constituting four research thrusts: (1) modeling multisensory integration, attention, and decision making, and the associated neural mechanisms; (2) machine-learning algorithms for high-dimensional multimodal data fusion; (3) adaptive tracking of the neural and behavioral models during online operation of the BCI; and (4) adaptive BCI control of multisensory cues for optimized performance. Complementary experiments with rodents, monkeys, and humans will be conducted to collect multimodal data to study and model multisensory integration, attention, and decision making, and to prototype a BCI for enhanced decision accuracy. The modeling efforts will span Bayesian inference, stochastic control, adaptive signal processing, and machine learning to develop: (1) novel Bayesian and control-theoretic models of the brain mechanisms; (2) new stochastic models of multimodal data and adaptive inference algorithms for this data; and (3) novel adaptive stochastic controllers of multisensory cues based on the feedback of users' cognitive state.

4. Realizing Cyber Inception: Towards a Science of Personalized Deception for Cyber Defense. This MURI began in FY17 and was awarded to a team led by Professor Milind Tambe at the University of Southern California. The goal of this MURI research is to gain scientific understandings to significantly advance the state of art in learning and modeling of adversarial mental states and decision processes, to create metrics quantifying information effectiveness in driving cognitive state change under the deception context, and to build an integrated framework of deception composition and projection methods to successfully manipulate adversaries' mental state and decision-making process to our advantages.

The research focuses on an innovative and comprehensive study of adaptive cognitive modeling, cyber deceptive game theory, and deception and monitoring systems that. The effort consists of three major thrusts: 1) Deception and Monitoring Systems: Ultimately deceptive strategies developed by higher-level reasoning about the attacker must be realized in a system, in such a way that the deceptions are convincing and their effects on the attacker can be effectively monitored. 2) Cyber Deceptive Game Theory: Game theory provides a mathematical framework for modeling the interactions between defenders and attackers in cybersecurity, which is an important foundation for developing a science of security. Developing game-theoretic models and algorithms for cybersecurity will allow richer modeling of adversarial interactions, a deeper understanding of deception and information manipulation tactics, and more effective response strategies. 3) Cognitive Modeling: Cognitive models provide a computational representation of human cognitive processes, their detailed mechanisms and limitations, and the knowledge upon which they operate. By taking advantage of human bounded rational decision behavior, where humans make decisions according to the constraints on the environment of their own cognitive limitation, the team will build a personalized model of adversary behavior.

5. Semantic Information Pursuit for Multimodal Data Analysis. This MURI began in FY17 and was awarded to a team led by Professor Rene Vidal of Johns Hopkins University. The goal of this research is to establish the theoretical foundation for context and principles of information physics for data analysis that provide an analytical framework and computation algorithms for the characterization, analysis and understanding of information content in multimodal data.

The proposed information-theoretic framework for characterizing information content in multimodal data combines principles from information physics with probabilistic models that capture rich semantic and contextual relationships between data modalities and tasks. These information measures will be used to develop novel statistical methods for deriving minimal sufficient representations of multimodal data that are invariant to some nuisance factors as well as novel domain adaptation techniques that mitigate the impact of data transformations on information content by finding optimal data transformations. The computation of such optimal representations and transformations for classification and perception tasks will require solving nonconvex optimization problems for which novel optimization algorithms with provable guarantees of convergence and global optimality will be developed. The uncertainty of such information representations derived from multimodal data will be characterized via novel statistical sampling methods that are broadly applicable to various representation learning problems. The information representations obtained from multiple modalities will be integrated by using a novel information theoretic approach to multi-modal data analysis called information pursuit, which uses a Bayesian model of the scene to determine what evidence to acquire from multiple data modalities, scales and locations, and to coherently integrate this evidence. The proposed methods will be evaluated in various complex multimodal datasets, including text, images, video, cellphone data, and body-worn cameras.

C. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY17.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY17, the Division managed one new-start STTR contract, in addition to active projects continuing from prior years. The new-start project consisted of one Phase II contract. This new-start contract aims to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY17 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Serving Institutions (HBCU/MSI) – New Starts

The HBCU/MSI program encompasses the (i) Partnership in Research Transition (PIRT) Program awards, (ii) DoD Research and Educational Program (REP) awards for HBCU/MSIs, and (iii) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY17, the Division managed two new REP awards, in addition to active projects continuing from prior years. In addition, proposals from HBCU/MSIs are often among the projects selected for funding by the Division (refer to the list of HBCU/MSI new starts in *CHAPTER 2, Section IX*.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY17.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY17, the Division managed seven new DURIP projects, totaling $1.5 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. Joint Federal/ARL-ARO Advanced Computing Initiative

The Advanced Computing Initiative (ACI) is an ongoing ARL-ARO joint venture with other agencies on energy efficient computing. Specifically, energy efficiency is now a primary constraint in designing new supercomputers. In order to provide robust performance, future systems will need to be able to dynamically trade off energy efficiency, performance, and reliability. Initiated in FY13, the ACI program's objective is to support research for enabling these tradeoffs and will run for four years at approximately $4 million/year. ARO is responsible for the program management and contracting duties. The ACI program has a close relationship to

ARL's High Performance Computing efforts and they offer potential cost savings and reliability benefits for the Army. The costs associated with consuming megawatts of electricity both directly and for the elaborate cooling systems to deal with the excessive heat supercomputers generate are becoming excessive. More important is the machine's reliability as more power to the system means more heat to the components, significantly increasing failure rates. Developing hardware and software infrastructure to increase performance while ignoring the effects on power consumption and reliability will not be feasible in the future. Seven grants have been awarded under the ACI program to teams composed of members from academia, industry and the national laboratories.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Computing Sciences Division.

A. Hybrid Spectrum Face Detection and Recognition

Professor Jingyi Yu, University of Delaware, Single Investigator Award

The goal of this research is to create a new collaborative, multi-spectrum sensing solution to achieve the capability to track, detect, and identify human targets in highly cluttered scenes under extreme conditions, such as in complete darkness or in the battlefield, which has been one of the primary tactical advantages in military operations. The effort focuses on utilizing computational imaging, together with illumination for effective eye localization to create a class of new 2D/3D computer vision techniques for robust face pose estimation, 3D face geometry reconstruction, and face detection and recognition.

In FY17, Professor Yu and his team established a hybrid sensing system with NIR sensors and LWIR sensor (see FIGURE 1). The system consists of 5 sub-systems: 1) image acquisition, 2) eye localization, 3) landmarks detection, 4) pose estimation, and 5) face frontalization. The first subsystem consists of a long-wave IR (LWIR) camera and a pair of near-infrared (NIR) stereo cameras that are attached to the left and right sides of the LWIR camera. The LWIR camera captures thermal face images of the person as the reliable sources for face identification. The two NIR cameras capture two pairs of stereo images, with and without "bright-eye" effect. This "bright-eye" effect is similar to a phenomenon in photography known as the "red-eye" effect, except that now only NIR spectrum is captured. Each NIR sensor in our hybrid sensing system is surrounded by a ring of NIR flash lamps to strategically capture the "bright-eye" effect of the human. The NIR flashes are triggered by our designed flash control system which makes the system covert. The second subsystem, eye localization, estimates 3D eye positions from the NIR stereo images, efficiently localizes the eyes on the thermal image, and generates valid thermal face bounding boxes that contain the eyes. These face bounding boxes are further tightened by our trained thermal face detector. The landmarks detection subsystem uses these face regions as input into our trained thermal facial landmarks detector which is a deep cascaded convolutional neural network. Combining thermal eyes locations with the detection results, totally 5 landmarks on the thermal image (2 from projecting 3D eye positions and 3 directly detected from LWIR images) are obtained. The pose estimation subsystem estimates the head pose based on these 5 landmarks by projecting a standard 3D head model to the thermal image and minimizing the total projection error of the landmarks. The last subsystem performs the thermal face pose correction and face frontalization using the matched points between the standard head model and the thermal query images via soft symmetry.

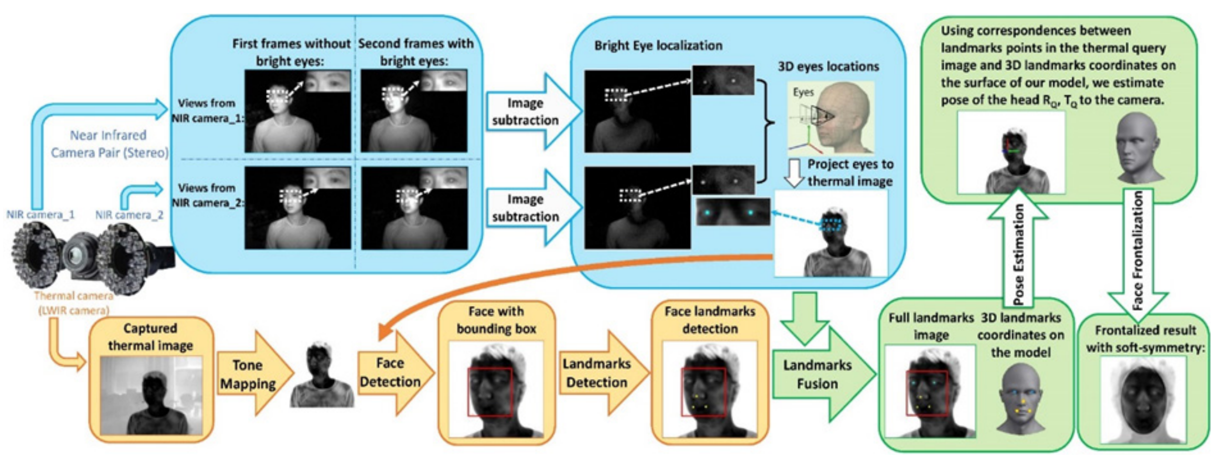

FIGURE 1

Illustration of proposed hybrid sensing system for face detection and pose standardization. The system consists of five sub-systems: 1) image acquisition, 2) eye localization, 3) landmarks detection, 4) pose estimation, and 5) face frontalization.

B. Mixed Reality for Managing Phantom Pain

Professor Balakrishnan Prabhakaran, University of Texas at Dallas, Single Investigator Award

The main aim of a project is to create a framework that can test the robustness of the data from 3D cameras. 3D cameras such as RGB-D (color + depth) and LiDAR (Light Detection and Ranging) cameras have enabled numerous computer vision applications such as crime scene reconstruction, damage detection, surveillance, autonomous vehicles etc. Tampering with data from 3D cameras may result in improper functioning of these applications. Therefore having the ability to detect tampering and being able to authenticate the data streams from 3D cameras is of great importance. In the course of this effort, this team discovered a way to apply their results to phantom limb pain management.

Phantom Limb Pain or simply Phantom Pain is a severe chronic pain that is experienced as a vivid sensation of the pain in missing body part. Epidemiological studies obtained from a large samples indicate that the short-term incidence rate of the phantom limb pain is 72%, while long-term incidence rate (6 months after amputation) is 67%. A wide spectrum of treatments developed for alleviating phantom limb pain includes recently developed virtual reality-based methods. Most of the virtual reality-based methods rely on 3D CAD models of the virtual limb, animating them using the motion data acquired either from patient's existing anatomical limb or myoelectric activity at the patient's stump (of the amputated limb). Since motion activity is typically captured using body sensors (Electromyography, EMG, or inertial sensors), these methods are considered as invasive approaches. Further, in the case of virtual reality-based methods, the dependency on the pre-built 3D models degrades the immersive experience due to a mismatch in the skin color, clothes, artificial and rigid look and misalignment of the phantom limb.

In FY17, this researcher and his graduate student developed a novel Mixed Reality based system for Managing Phantom Pain (Mr.MAPP), utilizing off-the-shelf RGB-D cameras such as Microsoft Kinect V2 to capture and generate a 3D model of the patient in real-time. An illusion of the virtual limb is crafted in real-time by mirroring the patient's symmetric anatomical limb in the captured data with the help of various computer vision and graphics techniques (see FIGURE 2). A phantom limb skeleton is also generated in real-time to enable interaction with virtual objects. A multi-pronged user Quality of Experience (QoE) study of Mr.MAPP was conducted employing various rendering displays such as 3D Television, and Head mounted displays (Oculus Rift, Samsung Gear VR). The user study involved two classes of users: (a) a big pool of Subject-Matter Experts (SMEs) that included Physical Medicine and Rehab experts, Amputee Occupational Therapists and Doctors of Chiropractic; and (b) healthy non-expert users. SMEs, as well as the healthy non-expert users provided extremely positive feedback of Mr.MAPP indicating the potential value of Mr.MAPP for phantom pain management.

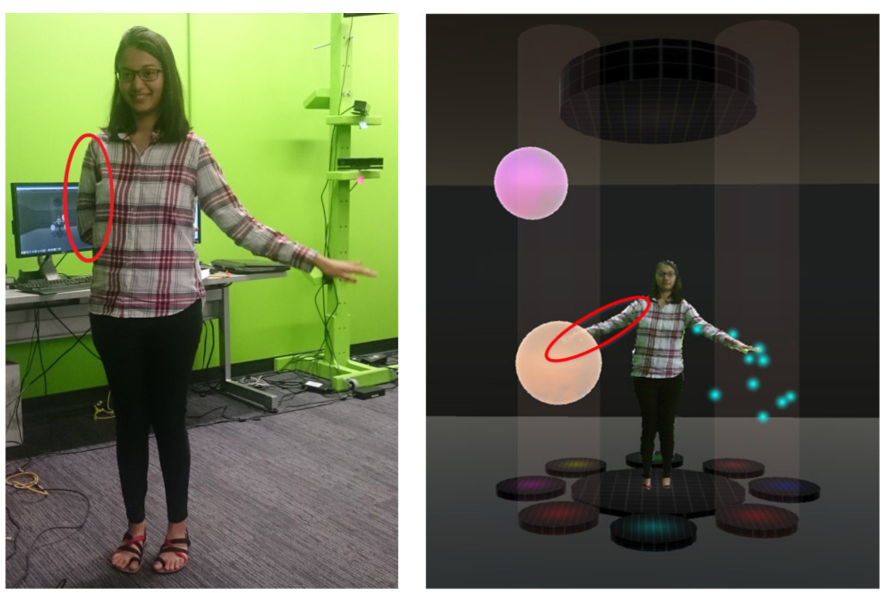

FIGURE 2

Phantom limb generation. Kinect is used to capture body data of a healthy person pretending to have a missing right arm and then Mr.MAPP is used to generate a virtual right arm. Left - real scene with healthy user keeping her right hand behind. Right - virtual scene with phantom limb generated by Mr.MAPP.

C. 3D Modeling of Urban Sites from Point Clouds

Professors Suay You and Ulruch Neumann, University of Southern California, Single Investigator Award

The objective of this research is to pursue new techniques and solutions that extend the range of urban object classes that can be rapidly processed and modeled from complex point-cloud data such as those collected from LiDAR scans. In particular, the team is pursuing an innovative modeling technique called Model By Recognition (MBR). MBR is a novel alternative to traditional modeling approaches that is an entirely new and promising approach for modeling a diversity of objects with arbitrary shape, layout, and surfaces in urban environments. The research foci are the MBR framework and its key components and technical barriers including point-cloud feature detection, recognition, shape matching, and 3D model generation. The research aims to provide solutions with significant advantages over current techniques, and add important new knowledge to the science of modeling of complex data and systems.

In FY17, the researchers developed a new technique for detecting, recognizing, and modeling pole-like urban object from 3D point clouds. Given a 3D point cloud representing the cluttered urban scenes, the technique can rapidly localize the pole-like objects in the point clouds, segment the objects out from backgrounds, infer their geometric structures and shapes, classify them to semantic labels, and then construct their 3D models representing as point clouds or polygon surfaces. Technically, there are three major stages of the processing. The first stage is localization, where all possible locations of pole-like objects are extracted from point clouds making use of the unique geometry and functionality characteristics of pole-like objects. The second stage is segmentation, in which the ground and other disconnected components are trimmed at the candidate locations. The method of 3D region growing is adapted to progressively segment out the objects from background. Finally, several statistical and geometrical attributes are computed for each candidate using the extended distribution features to classify the candidates with a Support Vector Machine (SVM) classification mechanism. The techniques were evaluated with various datasets (SEE FIGURE 3).

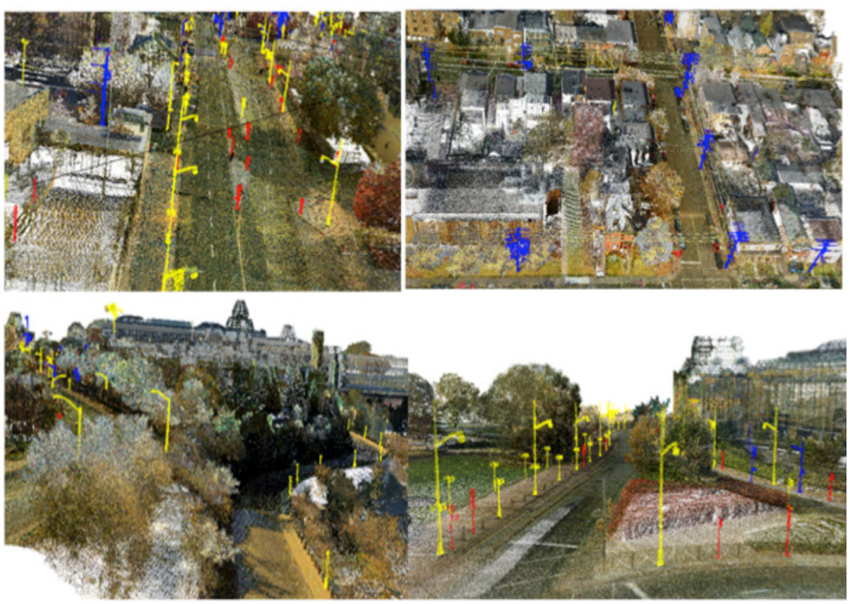

FIGURE 3

Detection and modeling results of Ottawa point cloud datasets. The input is a large-scale point cloud of an urban area from which a 3D model of the urban area is generated as depicted in the illustrations above. Then pole-like objects are detected and classified into three categories: street lights, utility poles, and signs. In the above illustrations street lights, utility poles, and signs are highlighted in yellow, blue, and red, respectively.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Efficient Computational Models for Simulating Large-Scale, Heterogeneous Crowds

Investigator: Professor Ming Lin, University of North Carolina - Chapel Hill, Single Investigator Award
Recipient: U.S. Army's Institute for Creative Technologies (ICT)

Understanding the behavior of pedestrians in a crowded scene has been the subject of extensive research in multiple domains, including applied mathematics, robotics, psychology, sociology, civil and traffic engineering, architectural and urban design, etc. Many applications such as training for battlefield simulation and urban warfare, intelligent surveillance, management of large mobs or unruly crowds, as well as use of robots in battlefields and dangerous environments need improved capabilities to simulate large crowds. Such crowds are characterized based on number of agents or pedestrians (e.g. large crowds with tens or hundreds of thousands of people), high densities, as well as heterogeneous or varying behaviors. Current state of the art is not able to model such large and diverse crowds that arise in different applications. Motivated by the practical demands of modeling and simulation and better understanding of dynamic aggregate behaviors that are observed in modern-day Megacities, the goal of this project is to develop novel computational models and real-time crowd simulation algorithms that can be used to for battlefield simulation, personnel training, and design evaluation.

In FY17, this researcher and her graduate student, in conjunction with researchers at the Army's Institute for Creative Technologies (ICT), developed a novel algorithm for generating virtual avatars which move like the represented human subject, using inexpensive sensors and commodity hardware. The algorithm is based on a perceptual study that evaluates self-recognition and similarity of gaits rendered on virtual avatars. First, discriminatory features of human gait are identified and then a data-driven synthesis algorithm generates a set of similar gaits from a single walker. These features are combined to automatically synthesize personalized gaits for a human user from noisy motion capture data (see FIGURE 4). The overall approach is robust and can generate new gaits with little or no artistic intervention using commodity sensors in a simple laboratory setting. These algorithms have been incorporated into ICT simulation systems and a joint publication was produced.

FIGURE 4

Generating crowds with diverse motions. Current animation systems often use a small set of template motions to animate large crowds, which can appear to be cloned or unnatural. Left - All avatars are animated with an identical gait, indicated by the perfect synchronicity in arm and leg movement across characters. Right - This approach generates personalized gaits for each virtual avatar, leading to diverse motion styles and natural appearing crowds.

B. Automated Evasive Malware Detection System Based on Transparent Dynamic Analysis

Investigator: Professor Giovanni Vigna, UC Santa Barbara, Single Investigator Award
Recipient: Air Force Life Cycle Management Center at Joint Base San Antonio - Lackland

A common shortcoming of current virtual machine based malware analysis and detection systems is that adversaries can detect the presence of virtual machines and avoid exhibiting malicious behavior to evade detection. An attacker can submit malware samples specifically designed to extract the malware analysis environment artifacts to be then used in fingerprinting the analysis system. Researchers at the University of California Santa Barbara have created an automated evasive malware detection method based on real hardware systems that can enhance warfighter capability in cyber defense. The new approach executes and analyzes malware samples on native hardware and compares their behavior to execution through emulation or on virtualization-based systems. This approach provides a robust transparent environment for the reference system where both user-mode and kernel-mode malware can be analyzed. By transparently extracting the behavioral profile of the malware from its disk-level and network-level activity, the true behavior profile of evasive malwares can be captured for detection. In FY17, the malware analysis software was transitioned to the Cyber Systems Division of the Air Force Life Cycle Management Center at Joint Base San Antonio-Lackland in San Antonio, Texas. The new capability will allow DoD cyber defenders to enhance their capabilities in defending against potential cyber threats by stopping incoming malwares before they can make damages to the mission.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Algorithms for Visualization and Simulation of Optimal Navigation

Professor Marcelo Kallmann, University of California at Merced, Single Investigator Award

This project will investigate new GPU-based algorithms for computing global and optimal navigation information in given environments, with the goal to introduce optimal metrics in multi-agent simulations and to develop new tools and analysis of navigation strategies. Because global navigation is strongly related to path planning, this project will develop new techniques for computing, representing, and visualizing globally optimal shortest paths in varied situations. The starting point for this project is the computation of Shortest Path Maps (SPMs), which are spatial decompositions that encode all the shortest paths in the plane relative to a source point defined in the environment (see FIGURE 5). SPMs are difficult to compute and this project will follow a GPU-shader programming approach that is capable of successfully generating SPMs of complexity not seen in previous work and will achieve new types of optimal path maps not previously addressed, enabling the computation of new path planning queries with optimality guarantees. This work will also develop novel approaches for introducing global optimality to the paths selected for each agent in a multi-agent simulation leading to multi-agent simulations based on clear metrics and thus more informative as support for strategic movement or space design decisions, such as planning exit points in evacuation plans. This project therefore has the potential to provide critical capabilities not previously addressed in simulation based navigation analysis and visualization. It is anticipated that in FY18, GPU-based algorithms will be developed to generate SPMs that allow modeling long entrances or exits while still keeping global optimality guarantees which will then be used to simulate and visualize multi-agent evacuation scenarios together with the computation of optimal navigation performance metrics.

FIGURE 5

Computation of Shortest Path Maps (SPMs). Left - SPMs provide a decomposition of the free space into regions of linear and/or hyperbolic boundary segments. Each region has a unique parent vertex, which is the first vertex to take for any point in the region to move along its globally shortest path to the source point. The shortest path (red line) between source point p and point q is illustrated in the figure. Right - SPMs enable the computation of distance fields, which encode the optimal distances from the source point to all points in the plane, achieving a global visualization of the accessibility to the different areas in the environment. The regions depicted in red are the ones most distant from the source point, an information easily observable from the distance field visualization.

B. Target Tracking and Recognition under Adverse Visual Conditions

Professor Ying Wu, Northwestern University, Single Investigator Award

Most contemporary computer vision techniques assume mild visual conditions and depend on good quality imagery. In practice, however, as the environments are unconstrained, their performances are largely jeopardized by *adverse visual conditions (*e.g., induced by bad weather conditions or imaging conditions), when the visual quality of the data is seriously degraded and the visual details may be obscured in such *perceptually ``low-quality" imagery*. Most existing solutions to this challenge are to perform pre-processing that restores the quality of the imagery, e.g., via image super-resolution, de-blurring or de-hazing. However, image restoration tasks themselves are very difficult and computationally demanding. Therefore, such a solution is not practical. Except some *ad hoc* methods, satisfactory solutions are still yet to be found, which has impeded the development of "all-weather" vision systems in practice. The objective of this project is to establish an innovative solution to overcome this challenge, by exploring a unified approach that does *not perform explicit image restoration* as pre-processing in performing target tracking and recognition tasks under various adverse visual conditions and degradations.

In FY18 this project will design a new computational model for handling low-resolution imagery for video-based target tracking and identification. It avoids performing the computationally demanding data pre-processing for visual restoration. It is a general approach of learning visual similarity that applies to various situations of adverse visual conditions. Research will also establish effective methods for target tracking and identification under low-resolution imagery. Based on a new metric steering approach, the metric of low-quality imagery can be learned, by steering and aligning the known similarity metric in good-quality images captured under mild visual conditions. This empowers computationally efficient target matching, tracking and identification.

C. Human-to-device (H2D) authentication

Professor Domenic Forte, University of Florida, Single Investigator Award

This project explores the new concept of "human-to-device" (H2D) authentication. H2D explicitly ties a system's operation to certain authorized personnel by combining biometrics with new system (PCB) level obfuscation approaches (see FIGURE 6). In H2D, connections between the chips on the PCB are obfuscated with permuting blocks/chips which are controlled by a key generated from a user's electrocardiogram (ECG). The ECG-based key is never stored on the device and can only be generated by supplying an ECG at the H2D interface. If an authorized ECG is applied, the connections between chips on the PCB will be correct and the system will be activated/unlocked. Otherwise, the system will be locked or nonoperational. Reconfigurable hardware can be added in order to update the obfuscation for different users (ECGs) over time. The use of ECG as a biometric guarantees with high confidence that the authorized person is present, thus providing authentication. Compared to other obfuscation approaches, the key provided by ECG is less vulnerable to theft, brute force attacks, cloning, and other forms of circumvention, thus making the system more robust against unauthorized access, reverse engineering, and cloning if captured by an enemy. This represents a significant advancement over the state-of-the-art and could have a substantial impact on DoD core missions. The researcher will evaluate the quality (uniqueness, reliability, and cost) of ECG-based keys and explore opportunities for system (PCB) level obfuscation based on permutation and evaluate them in terms of security and cost. In FY18, the researcher will develop metrics for permutation-based obfuscation at system level and evaluate the uniqueness of ECG-based keys. In addition new research effort will augment existing synthetic ECG models with statistical models that capture the dynamics of sympathetic processes, parasympathetic processes, physical activities, noise, etc. on ECG morphology.

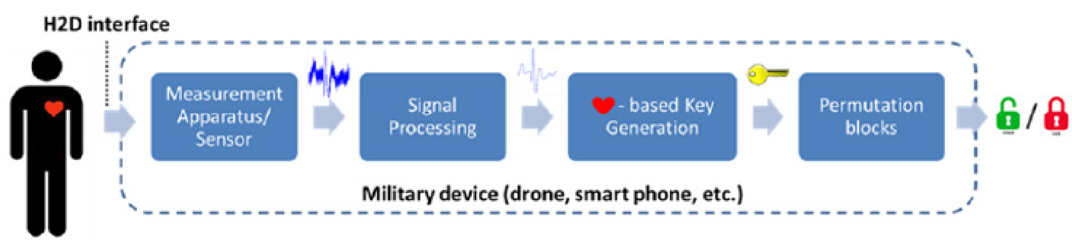

FIGURE 6

The ECG of a person is measured by sensors connected to the military device (drone, rugged computing device, etc.). The signal is processed and used to generate a key. The key unlocks the obfuscated PCB (allowing the device to operate) as long as it is the same as the one registered to the device. Otherwise, the device remains locked.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Cliff Wang
Division Chief
Program Manager, Information and Software Assurance

Dr. Mike Coyle
Program Manager, Computational Architectures and Visualization

Dr. Liyi Dai
Program Manager, Information Processing and Fusion

B. Directorate Scientists

Dr. Randy Zachery
Director, Information Sciences Directorate

Dr. Bruce West
Senior Scientist, Information Sciences Directorate

Ms. Anna Mandulak
Contract Support

C. Administrative Staff

Ms. Debra Brown
Directorate Secretary

Ms. Diana Pescod
Administrative Support Assistant

CHAPTER 5: ELECTRONICS DIVISION

I. OVERVIEW

As described in *CHAPTER 1*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2017* is to provide an annual historical record summarizing the programs and basic research supported by ARO in FY17. ARO's mission is to support creative basic research resulting in new science that enables new materials, devices, processes, and capabilities for the current and future Soldier. This chapter provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions enabled by the ARO Electronics Division in FY17.

A. Scientific Objectives

1. Fundamental Research Goals. The principal objective of research in the ARO Electronics Division is to discover and control phenomena that involve charged particles and waves in solid state materials and plasma. More specifically, the Division supports basic research to discover and control stimulus-response properties of electronic materials/structures, to leverage nanotechnology for enhanced electronic properties, to comprehend and mitigate distortion and noise, to understand and exploit complex electromagnetic and acoustic phenomena and propagation, and to explore ultra-fast, solid state and plasma mechanisms and concepts. The results of this research will stimulate future studies and help keep the U.S. at the forefront of research in electronics by revealing new pathways for the design and fabrication of novel electronic structures that have properties that cannot be realized with current technology.

2. Potential Applications. Electronics research is relevant to nearly all Army systems; therefore, research under this program provides the underlying science for a wide variety of developmental efforts and contributes to the solution of technology-related problems throughout the full spectrum of the Army's "System of Systems." Army-relevant research in electronics spans areas such as (i) nano- and bio-electronics to provide components that interface with biological systems, enhance the creation and processing of information, and require less power (ii) studies in electromagnetics, acoustics, microwaves, and power to enable multimodal sensing for detection, identification, and discrimination of environmental elements critical to decision-makers in complex, dynamic areas , including defeat of electronic threat systems, (iii) optoelectronics, which involves the creation and use of electromagnetic radiation from far infrared to X-ray for sensing, communication as well as countermeasures to interrogate, disrupt, and defeat hostile infrared sensor systems and (iv) action-reaction relationships in electronic materials and structures that may lead to new devices and methods for sensing and communication over long ranges and within complex environments.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Electronics Division coordinates and leverages research within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the Defense Advanced Research Projects Agency (DARPA), as well as the various DOD Labs and other governmental activities with electronics research missions. Moreover, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, sensing is a research element of all ARO Divisions, and the Electronics Division serves as the focal point for ARO sensing research. Specific interactions include joint projects with the Physics Division that promote research for physics-based understanding of semiconductor materials, non-reciprocal materials and devices, propagation effects, plasma devices, and stimulus response effects in condensed matter. The Electronics Division also coordinates its research portfolio with the Materials Science Division to pursue the design and characterization of new materials and structures, the evaluation of electrical properties, and the study of electronic processes at the molecular level. This Division complements its research initiatives in the Chemical Sciences Division to include research to understand how chemical changes and chemical structures influence electrical, magnetic, and optical properties and investigations of high frequency spectroscopic techniques for use in chemical defense, and explosive detection. The Life Sciences Division's Program Areas also interface with electronics research in areas of biological detection as well as interfacing to biological organisms. Lastly, creating computational methods and models for target recognition and understanding nano-molecular structures and carrier transport shared research goals between the Electronics and Information Sciences Divisions.

The Division's research portfolio will also reveal previously unexplored avenues for new Army capabilities while also providing results to support the ARL ERAs of (i) Intelligent Teams, (ii) Impact of Operating in a Contested Environment, and (iii) Implementation. In addition, the Division supports almost all of the other ARL S&T Campaigns, particularly the Materials Research Campaign which is supported by all of the Division's sub-areas with novel electronic and photonic materials. The Computational Sciences Campaign is supported through novel Nano, Bio, and Optoelectronic computing, Sciences-for-Maneuver by active and passive sensing, Information Sciences by new algorithms from biosciences as well as electromagnetic discoveries, Sciences for Lethality and Protection through targeting and directed energy, and Human Sciences through understanding and interfacing electronically with biological systems. The Electronics Division had 7 active cooperative agreements with these campaigns including a new cooperative agreement between the Materials Research Campaign and the State University of New York at Stony Brook to create novel metamorphic III-V narrow band structures.

B. Program Areas

The Electronics Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY17, the Division managed research within four Program Areas: (i) Nano- and Bio-electronics, (ii) Electromagnetics and Radio Frequency Electronics, (iii) Optoelectronics, and (iv) Electronic Sensing. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have long-term objectives that collectively support the Division's overall objectives.

1. Nano- and Bio-electronics. The program focuses on the creation of novel electronic devices including nano- and bio-based sensors and transducers based on semiconductor electronics and hybrid molecular-semiconductor devices in addition to organic-inorganic hybrid materials. This project supports basic research that will apply biology concepts to electronics and photonics to create biomimetic structures and devices for information processing, information storage, electronic components, and actuators. It will also create unique electronic sensors at the nano to the macro level that interface with biological materials in order to extract information on biological systems. The long term goal of this task is to discover and control novel phenomena by the combination of electronics, photonics, and bioscience to provide novel electronic technological capabilities for defense-related applications such as sensing, data processing, communications, target recognition, navigation, and surveillance.

2. Electromagnetics and Radio Frequency Electronics. This program area is concerned with investigation of electromagnetic (EM) and radio frequency (RF) phenomena for integrated antenna arrays, multifunctional antennas, EM power distribution, and new sensing modalities. It also explores acoustic phenomena and new concepts for circuit integration for greater functionality, smaller size/weight, lower power consumption, enhanced performance, with focus in the frequency regime from low to terahertz frequencies.

This area addresses the science behind new approaches to the generation, transmission, and reception of EM power and signals. Emphasis is placed on the HF through terahertz spectrum, however, novel ideas at lower frequencies down to direct current may be addressed. In the RF regime orders of magnitude improvements in systems performance, cost, weight, reliability, size characteristics, and functionality will be sought. Issues include the coupling of EM radiation into and out of complex structures, antennas, both active and passive, transmission lines and feed networks, power combining techniques, EM wave analyses of electrical components, and EM modeling techniques. Thermal problems stemming from the concentration of higher and higher power into smaller and smaller volumes will be addressed. Antenna research will break away from the methodologies that were developed for continuous-wave, narrowband, steady-state operation to invent new design techniques, architectures, and materials that can dramatically increase the radiation efficiency and bandwidth of tactical antennas while simultaneously reducing their size and signature. The EM and acoustic detection and analysis of underground targets, landmines, and IED's will continue to be of interest. Unusual propagation effects in the atmosphere and gaseous plasmas offer new opportunities for sensing and detection. Army applications of this technology include communications (both tactical and strategic), command and control, reconnaissance, surveillance, target acquisition, and weapons guidance and control.

3. Optoelectronics. The goal of this Program Area is to discover and control novel nanostructure and heterostructure designs for the generation, guidance, and control of optical/infrared signals in both semiconductor and dielectric materials. The research in this program may enable the design and fabrication of new optoelectronic devices that give the Soldier high-data-rate optical networks including free space/integrated data links, improved IR countermeasures, and advanced 3D imaging. This program has three Thrust areas: (i) High Speed Lasers and Interconnects, (ii) Ultraviolet and Visible Photonics, and (iii) Mid-infrared Lasers. The research topics seek to overcome slow spontaneous lifetimes and gain dynamics, low carrier injection efficiency, poor thermal management, and device size mismatches. Novel light emitting structures based on III-V compounds, wide bandgap II-VI materials, rare-earth doped dielectrics, and silicon nanostructures are being investigated along with advanced fabrication and characterization techniques. Nanotechnology is exploited to allow interfacing of optoelectronic devices with electronic processors for full utilization of available bandwidth. Electro-optic components are being studied for use in guided wave data links for interconnections and optoelectronic integration, which are all requirements for high speed full situational awareness. In addition, emitters and architectures for novel display and processing of battlefield imagery are also important.

4. Electronic Sensing. The goal of this Program Area is to extend the underlying science behind action-reaction relationships in electronic materials and structures as well as understand target signatures. This Program Area is divided into two research Thrusts: (i) Photonic Detection and (ii) Thermal, Mechanical, and Magnetic Effects. The scientific objective of Photonic Detection is to understand and control the direct conversion of light to charge in infrared materials and structures. This includes the design and fabrication of novel detector structures, such as superlattice or barrier structures, as well as novel plasmonic effects. An important element in this thrust area is the reduction of performance limiting defects in semiconductor material and structures through lattice matching and other methods. Development of novel characterization techniques is also explored to determine the fundamental issues behind carrier transport, lifetimes, and noise. The Thermal, Mechanical, and Magnetic Effects Thrust includes the modalities of acoustic, magnetic, infrasound, as well as thermal effects for infrared detection. Research in this Program Area seek to give the Soldier 100% situational awareness of vehicles, personnel, weapon platforms, projectiles, explosives, landmines, and improvised explosive devices (IEDs), in day/night, all weather, and cluttered environments through natural and man-made obstructions.

C. Research Investment

The total funds managed by the ARO Electronics Division for FY17 were $22.4 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY17 ARO Core (BH57) program funding allotment for this Division was $7.2 million and $1.3 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $2.5 million to projects managed by the Division. The Division also managed $1.8 million of Defense Advanced Research Projects Agency (DARPA) programs, and $4 million provided by other Federal agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $4.7 million for contracts. In addition, $1.9 million was provided for awards in the Historically Black Colleges and Universities and Minority Serving Institutions (HBCU/MSI) Programs, including funding for DoD-funded Partnership in Research Transition (PIRT), DoD-funded Research and Educational Program (REP) projects, and $1.0 million of the Division's ARO Core (BH57) funds, with the latter included in the BH57 subtotal above.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY17 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY17 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY17, the Division awarded 16 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Ritesh Agarwal, University of Pennsylvania; *Engineering the Properties of Orbitronic Nanomaterials*
- Professor Levon Asryan, Virginia Polytechnic Institute & State University; *Quantum Dot Lasers with Asymmetric Barrier Layers: A Novel Type of Semiconductor Lasers*
- Professor Seth Bank, University of Texas at Austin; *Staircase Avalanche Photodiodes*
- Professor Rodrigo Amezcua Correa, University of Central Florida; *Antiresonant Hollow Core Fibers for Extreme Light Propagation*
- Professor Dirk Englund, Massachusetts Institute of Technology (MIT); *High-Quality Tunable Graphene Plasmonic Metamaterials*
- Professor Milton Feng, University of Illinois - Urbana – Champaign; *Ultrafast Directly Current and Tunneling Modulated Microcavity Laser (DML) toward10 fJ/bit and > 100Gb/s Optical Networks*
- Professor Dejan Filipovic, University of Colorado – Boulder; *Full Duplex Antenna Study*
- Professor Philip Kim, Harvard University; *Hydrodynamic Electron Transport in 2-Dimensional Materials for Nanoelectronics*
- Professor Keji Lai, University of Texas at Austin; *Near-field Microwave Probing of Nontrivial Topological Boundary States*
- Professor Guifang Li, University of Central Florida; *Beamforming Techniques for Focusing Light Through Atmospheric Turbulence*
- Professor Zetian Mi, University of Michigan - Ann Arbor; *Electrically Injected 280 nm AlGaN Nanowire Edge-Emitting Lasers*
- Professor Jagdish Narayan, North Carolina State University; *Doping of Diamond and c-BN beyond Thermodynamic Solubility Limit for Solid State Devices*
- Professor Daniel Sievenpiper, University of California - San Diego; *Acoustic/Phononic Topological Insulators Using Complementary Conductors*

- Professor Lan Yang, Washington University; *A versatile photonic platform for sensing and beyond*
- Professor Zhi-Gang Yu, Washington State University; *Electronic Sensing: Characterization, Modeling, and Optimization of Cross-Linked Metal Particles for Microbolometers*
- Professor Xi-Cheng Zhang, University of Rochester; *Extreme THz Science*

2. Short Term Innovative Research (STIR) Program. In FY17, the Division awarded 7 new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Vitaly Kresin, University of Southern California; *Size-selected nanocluster particles as novel building blocks for high-Tc superconducting systems*
- Professor Guifang Li, University of Central Florida; *Towards AO-Free FSO Communication*
- Professor Zetian Mi, University of Michigan - Ann Arbor; *Molecular Beam Epitaxial Growth and Characterization of Two-Dimensional BN/MoxW1-xSe2 Heterostructures*
- Professor Zetian Mi, University of Michigan - Ann Arbor; *Molecular Beam Epitaxial Growth of InGaN/GaN Dot-in-Nanowire Heterostructures*
- Professor Winston Schoenfeld, University of Central Florida; *Solar Blind Sn-alloyed Ga2O3 Schottky Photodetectors*
- Professor Michael Stroscio, University of Illinois – Chicago; *Nanomechanical Systems with Normalized and Coupled Acoustic and Electromagnetic Modes in Piezoelectric Structures*
- Professor Peide Ye, Purdue University; *Isolation of a Single Tellurium Atomic Chain*

3. Young Investigator Program (YIP). In FY17, the Division awarded one new YIP project to drive fundamental research in an area relevant to the current and future Army. The following PI and corresponding organization was the recipient of a new-start YIP award.

- Professor Jacob Adams, North Carolina State University; *Reconfigurable Electrofluidic Networks for Highly Adaptive Electronic Warfare Platforms*

4. Conferences, Workshops, and Symposia Support Program. The Division provided funds in support of a range of scientific conferences, workshops, and symposia that were held in FY17. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences, with the goal of supporting scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army, and to define the research needs, thrusts, opportunities, and innovation crucial to the future Army. Proposals requesting funding support, typically for less than $10K, were received and evaluated in line with the publicly available ARO BAA. In FY17, five proposals were selected for funding by the Division to support FY17 conferences, workshops, or symposia.

5. Special Programs. In FY17, the Division also awarded six new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school and undergraduate students. These efforts were funded through the ARO Core Program and Youth Sciences Programs, for research to be performed at academic laboratories currently supported through active SI awards (refer to CHAPTER 2, Section IX).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Electronics Division; therefore, all of the Division's active MURIs are described in this section.

1. Near and Far-Field Interfaces to DNA-Guided Nanostructures from RF to Lightwave. This MURI began in FY10 and was granted to a team led by Professor Peter Burke at the University of California - Irvine. The goal of this research is to develop new sensing modalities for chem/bio sensing based on materials development in nanotechnology and nanoscience, and to interface nano-electronic and nano-optical components to biologically relevant physical properties.

In order to tap the requisite contributions from different academic disciplines (DNA chemistry, electrophysiology, nano-electronics, optics and THz spectroscopy), three sensing hardware testbeds are being developed for further testing, functionalization, and analysis: (i) bottom up carbon electronics (graphene, nanotubes); (ii) top down silicon nano-electronics (top down Si nanowires); and (iii) nano-optics (CdSe and other nanowire emitter/detector architectures). Two functionalization schemes are being be applied to these testbeds to enable sensing: DNA origami aligned to nanowire arrays and ion channel functionalization for electrophysiology at the nanoscale. Unique aspects of this sensing research include multiplexing (massively parallel sensor arrays) via DNA self-assembly. Using this approach, in principle, each nanowire in an array can have a different sensing functionality, at unprecedented pitch. In addition, direct integration of bio-electrical signals (ion channel currents) to nano-electrodes (carbon, silicon, and nano-optics) are being explored. A key discovery in the recent year is that the ion channel current pulses can be used to charge the quantum capacitance of graphene, demonstrating a qualitatively new sensing modality for nanoscale electrophysiology. Lastly, single-molecule sensitivity and novel mechanisms for selectivity at THz frequencies are being pursued. Advances in this MURI will enable a new class of sensors for applications in biomedical diagnostics for civilian and warfighter health care, chemical agent detection, nano-optical devices for sensing, and neural-electrical interface at unprecedented spatial resolution.

2. Defect Reduction in Superlattice Materials. This MURI began in FY11 and is led by Professor J. M. Zuo at the University of Illinois - Urbana Champaign. The team consists of researchers from Arizona State University, Georgia Tech, and the University of North Carolina - Charlotte. The objective of this project is to determine and understand the relationship between minority-carrier lifetimes and classes of defects in superlattice materials and to formulate strategies for growth and post processing to eliminate or mitigate defects.

This research effort includes an in-depth study of the origins and structural, electrical and optical properties of defects, in-situ and ex-situ probing of defects during growth and fabrication, an investigation of defect reduction techniques, a study on ways to minimize the impact of defects on performance, and testing of results through fabrication and characterization of superlattice structures and devices. Understanding defects at the basic level in these superlattice materials will promote advancements in lasers and modulators as well as infrared detectors. For detectors, lifetime improvements will allow the next generation of focal plane arrays with increased long wave resolution, much larger array formats, broader spectral range into the very long wave infrared, and higher operating temperature to reduce life cycle costs.

3. Spin Textures and Dynamics Induced by Spin-Orbit Coupling. This MURI began in FY16 and is led by Professor Kang Wang at University of California, Los Angles. The team consists of researchers from University of California, Irvine, California Institute of Technology, University of Nebraska, North Carolina State University, and University of Texas, Austin. The objective of this project is to strive for understanding of interfacial spin-orbit coupling (SOC) and exchange coupling in novel heterostructures and superlattices of topological insulators (TIs), 2D transition metal di-chalcogenides (TMDs), and ferro-(FM)/ferri-/antiferro (AFM)-magnetic materials. High quality heterostructures and superlattices containing TI/TMDs, TI/FM, and TI/AFM with the atomically sharp interface are to be synthesized and characterized, and these will constitute an ideal laboratory for enabling understanding of the interfacial SOC effects and relevant spin textures and dynamics.

This project will exploit the symmetry breaking and SOC-induced collective properties (i.e., magnetization, spin wave, and spin-orbit torque) in these heterostructures and superlattices to realize new types of topological matters such as magnetic Skyrmions, topological valley insulators, and topological spin wave (magnonic) crystals. It will also help facilitate the development of new emerging fields including spin-orbitronics, spin-valley-tronics, and axion electrodynamics. In addition, direct electrical field manipulation of spin or magnetization textures in these proposed systems through spin-orbit torque and magnetoelectric effects will be investigated for energy efficiency. The anticipated results of this project will broaden understandings of the fundamental science enabled by SOC, and establish suitable material frameworks for new spin-orbitronic devices in which multi-functional applications of spintronics for ultra-low power electronics at terahertz can be realized. This research will set a milestone in the spin-based applications by creating the knowledge base to enable novel, fast, and energy efficient technologies for communications and information processing.

C. Small Business Innovation Research (SBIR) – New Starts

Research within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY17, the Division managed eight new-start SBIR contracts, in addition to active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY17 and prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY17, the Division managed nine new-start STTR contracts, in addition to active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY17 and a list of prior-year topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Serving Institutions (HBCU/MSI) – New Starts

The HBCU/MSI program encompasses the (i) Partnership in Research Transition (PIRT) Program awards, (ii) DoD Research and Educational Program (REP) awards for HBCU/MSIs, and (iii) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY17, the Division managed five new REP awards, in addition to active projects continuing from prior years. In addition, proposals from HBCU/MSIs are often among the projects selected for funding by the Division (refer to the list of HBCU/MSI new starts in *CHAPTER 2, Section IX*.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY17.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY17, the Division managed 8 new DURIP projects, totaling $1.5 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. JTO Multidisciplinary Research Initiative (MRI) Programs in High Energy Lasers

ARO currently manages eight MRI programs for the High Energy Laser Joint Technology Office (HEL-JTO) in Albuquerque (managed by OSD). Five of those are 2012 start MRIs and three of those were awarded through ARO's Electronics Division (the others through Materials and Physics). The three 2010 starts MRI are led by professors at Clemson University, the University of New Mexico, and the University of Central Florida. The latter two ended in FY16; whereas, the Clemson effort was extended an additional 2 years to further study the potential of all-solid photonic bandgap fibers. The two that ended were on high energy laser coatings and characterization techiques, and volume Bragg gratings. The 2012 start MRIs that are still active are led by professors at Rutgers, Texas Tech, University of California – Riverside, Clemson, and the University of Central Florida (Center for Research in Electro-Optics and Lasers). These MRIs are on the following topics: single crystal fiber lasers, rare-earth doped GaN, polycrystalline AlN ceramic gain media, leaky wave and gas-filled hollow-core fiber lasers, and nonlinearity mitigation in fiber lasers. The 2012 start MRIs are all in the final two years. ARO continues to play a significant role in leading the MRI programs by organizing kickoff meetings and program reviews, particularly in conjunction with the HEL-JTO Advanced Concepts Technical Area Working Group which leads the more basic research endeavors that HEL-JTO supports. The ARL Materials Science Campaign (ARL-CISD and ARL-SEDD) participate in HEL-JTO program evaluation through annual reviews.

I. DARPA Advanced Wide FOV Architectures for Image Reconstruction and Exploitation (AWARE)

The AWARE program focuses on technologies to enable wide FOV, higher resolution and multi-band imaging for increased target discrimination and search in all-weather day/night conditions. The Electronics Division coordinates research with this program by identifying and monitoring basic research projects with complementary goals. In FY16, the AWARE program provided new funding for four university projects because of ARO's leadership in the area of infrared photodetectors. In one, the objective is to create low-cost zero-dimensioned nanostructure-contained quantum disks that can be integrated into uncooled LWIR focal plane arrays. Another will demonstrate that the extreme mobility of CdO will enable plasmonic uncooled mid-infrared detectors. The third will determine the causes of Random Telegraph Noise and use that information to design read out integrated circuits in advanced fabrication nodes. The fourth will create and test efficient modulators that can achieve over 1 GHz bandwidth for SWIR (short wave infrared) Time of Flight (ToF) imaging. These follow ARO MURIs on quantum dot photodetectors and uncooled thermal materials as well as single investigator projects on noise and plasmonic enhancements for better photonic properties.

J. DARPA Low Cost Thermal Imaging – Manufacturing (LCTI-M)

The Low Cost Thermal Imager - Manufacturing (LCTI-M) program seeks to enable widespread use of infrared imaging technology by individual warfighters and insertion in small systems. The Electronics Division coordinates research with this program by identifying and monitoring basic research projects with complementary goals. In FY16, the LCTI-M program provided additional funding for an ongoing project to create free standing bolometer structures with thinner layers, lower heat capacity, and improved imaging performance over existing structures by use of atomic layer deposition. This was a joint project with the University of Colorado and DRS Technologies. ARO is the technical monitor for this project because of its leadership of an ARO MURI concerning uncooled materials.

K. DARPA Efficient Linearized All-Silicon Transmitters ICs (ELASTx) Program

The goal of the ELASTx program is to enable monolithic, ultra-high power efficiency, ultra-high linearity, millimeter-wave, silicon-based transmitter integrated circuits (ICs) for next-generation military microsystems in areas such as radar and communications. The ARO Electronics Division currently co-manages two university grants within this program that are exploring quasi-optical power combining of Doherty amplifiers, and asymmetric multilevel outphasing of large numbers of transistor amplifiers. The program will lead to revolutionary increases in power amplification efficiency while simultaneously achieving high linearity for digitally modulated signals. Prototype ELASTx amplifiers are being tested by scientists in ARL-SEDD for potential use in Army radar and communications systems.

L. DARPA High Frequency Integrated Vacuum Electronics (HiFIVE) and THZ Electronics Programs

The long-term vision for the DARPA THZ Electronics program is to develop the critical device and integration technologies necessary to realize compact, high-performance electronic circuits that operate at center frequencies exceeding 1012 cycles per second (i.e., 1 THz). The DARPA HiFIVE program will develop a compact, efficient source of electromagnetic energy capable of generating 100 W with 5 GHz bandwidth at 220 GHz using innovative cold cathode and micromachining technologies. The ARO Electronics Division and ARL-SEDD Electronics Technology Branch co-manage projects within these programs with a goal of using silicon micromachining and MEMS processes to produce precision interaction structures scaled for these extremely small wavelengths. These programs have a high potential impact on military communications, ECM, and radar systems. Two of the HiFive projects managed by ARO have now ended.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Electronics Division.

A. Carbon Nanotube Based Transistors Exceed Performance of Silicon

Professor Michael Arnold, University of Wisconsin - Madison, PECASE Award

Semiconducting carbon nanotubes (CNTs) offer a unique combination of exceptional electronic properties and excellent integrability. CNTs are expected to outperform leading electronic materials including silicon, gallium arsenide, and state-of-the-art thin films in field effect transistors (FETs) because of their exceptional charge transport properties; while at the same time, CNTs can be solution-processed and deposited onto almost any substrate, including plastics and fabrics. However, challenges have obstructed the tremendous promise of CNTs in electronics for more than two decades. Specifically, the primary challenges have been: (1) sorting semiconducting and metallic CNTs; (2) aligning semiconducting CNTs into tightly packed but well-spaced arrays; and (3) forming low-resistance electrical contacts to CNTs in FETs. In a recent paper in *Science Advances*, Professor Arnold and collaborators demonstrated that they had overcome these challenges to realize CNT-based FETs with higher performance than silicon and gallium arsenide FETs, for the first time, with 30-100*x* higher on-state conductance than previous CNT FETs at an on/off ratio of > 10^5 (see FIGURE 1). This advance was achieved by: (i) exploiting discovered structure-processing relationships that enable the selective binding of conjugated polymer wrappers to semiconducting CNTs and the elimination heterogeneous metallic CNTs to <0.01% abundances, (ii) leveraging a scalable, multi-phase fluid flow assembly process for depositing aligned arrays of CNTs on substrates at the intermediate packing density needed for high-performance FETs; and (iii) conducting post-deposition treatment to remove spurious adsorbates from CNTs that otherwise interfere with electrical contacts.

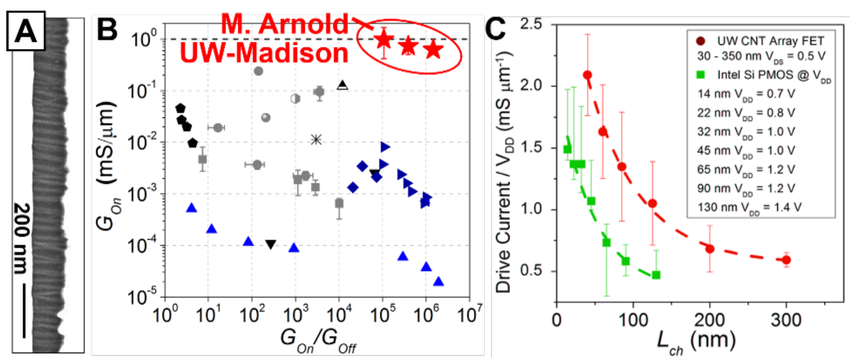

FIGURE 1

Analysis of semiconducting CNTs assembled into tightly packed but well-spaced arrays. (A) Electron micrograph of CNT array spanning Pd source and drain electrodes in a CNT array FET. (B) Arnold's CNT array FETs (circled) significantly outperform previous CNT FETs, considering two critical metrics: small bias on-conductance per width (y-axis) & on/off ratio (x-axis). CVD, solution-aligned, and randomly aligned FETs from literature are labeled black, grey, and blue, respectively. (C) On-current normalized by VDD versus channel length of Arnold's CNT FETs (red) versus Intel Si PMOS FETs (green).

B. Table Top Source of Bright, Coherent X-rays: The Ultraviolet Surprise

Professor M. Munane, University of Colorado - Boulder, Single Investigator and DURIP Awards

The goal of this research is to advance the state of technology for producing bright, coherent X-rays from a table top apparatus using extreme High Harmonic Generation (HHG). HHG from a plasma created by an ultrashort pulse laser (uspl) (pulse length hundreds of femtoseconds) has been demonstrated to generate broadband continuum, coherent radiation in the extreme ultraviolet wavelength range.

Previous research by the PI (supported by ARO) has shown that the radiation can be extended into the soft X-ray regime (up to 2 keV demonstrated) by driving the plasma with a mid-IR (~4 micron) uspl. The reason for this is that the extreme HHG process consists of an electron being ionized by the extreme field, which is accelerated away from the ion during half the laser cycle and returning to recombine with the atom on the reverse half cycle. The longer driving wavelength provides a longer time for acceleration of the electron and therefore more energy released on recombination. Theoretical calculations predict that this process can be used to generate up to 10 keV X-rays with longer wavelength lasers. The resulting X-rays must be phase matched with the driving field in order for coherent build-up of the X-ray field to take place. For mid-IR lasers, the window for phase matching is on the order of half a driving laser cycle. The UVt surprise is the discovery that an UV driving laser results in a regime with major advantages over the mid-IR driving lasers. The UV laser pulse results in less time the electron spends away from the parent ion, with less quantum diffusion. Furthermore, the higher linear and non-linear indices of the atoms and ions in the plasma counteract the plasma (electron) dispersion (see FIGURE 2), together with low group walkoff, resulting in a much longer phase matching window (many laser cycles). Although the X-ray energy range is less than for the longer wavelength driving lasers, the UV driven process is several orders of magnitude brighter with higher conversion efficiency and still reaches into the soft X-ray regime. The longer phase matching window can result in well-separated narrowband peaks (~9 eV separation with linewidths of 70-700 meV) (see FIGURE 3). The emission form, narrowband peaks or supercontinuum, can be controlled by the nature of the driving field (e.g., single or multiple wavelength, multiple propagation angle). Simulations show that the UV-driven HHG process can extend into the multi-keV regime and can produce a near time-bandwidth limited series of 100 attosec pulses. The resulting coherent X-rays have the ability to track electron dynamics in detail in atoms, molecules, materials, magnetic excitations, and phonons, with applications in developing new electronic and magnetic materials and devices.

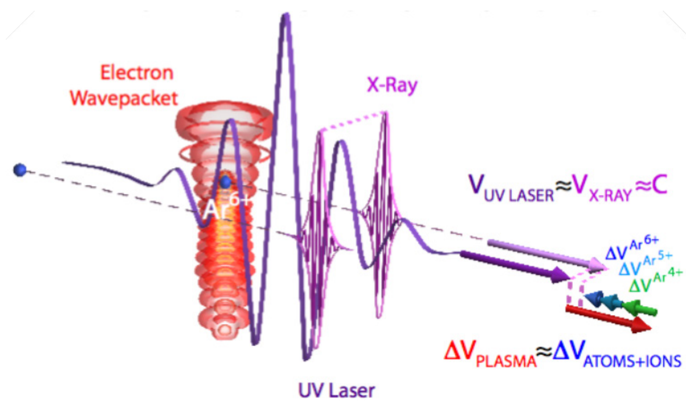

FIGURE 2

Electron wavepacket driven by UV uspl, interacting with Ar ion, producing X-ray field. The change in velocity due to the plasma dispersion (red arrow) is balanced by the change in velocity due to the dispersion from the ions and atoms (blue and red arrows). The result is that the velocity of driving UV field is nearly equal to the velocity of the resulting X-ray field, allowing the X-ray to build coherently.

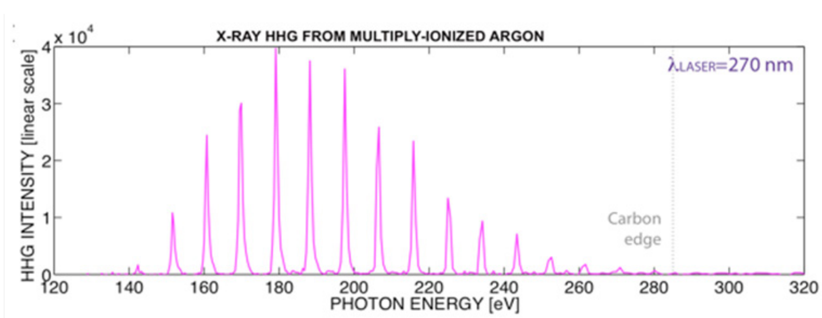

FIGURE 3

Narrowband X-ray peaks produced by HHG using UV driving uspl.

C. Advances in Gas Based Polariton Condensates Exceed Several Prior Limits

Professor David Snoke, University of Pittsburgh, Single Investigator Award

This research effort involves three groups: Profs. David Snoke, Pittsburgh, Allan MacDonald, Texas, and Loren Pfeiffer, Princeton and is funded jointly thru the Electronics and Physics Divisions. These studies focus on polariton condensates in GaAs/AlGaAs microcavities fabricated by collaborator Loren Pfeiffer. Prior work had already shown that they can reliably produce Bose-Einstein condensates of polaritons, and that the lifetime of the polaritons in these structures is several hundred picoseconds (corresponding to a Q-factor over 300,000), allowing excitonic transport distances of hundreds of microns to millimeters. The polariton condensates emit coherent light like a laser, but rely on the high nonlinearity of the system rather than inversion to reach this. There were three noteworthy accomplishments for FY17 within this one project:

1. Ultra-high nonlinearity in pillar structures. Initial work in this project showed the ability to create condensates in an etched pillar structure, and that the condensate can be trapped about 50 microns from the laser excitation spot. Because the condensate is so far from the pump spot, there is almost zero background light from the pump laser. This allows nonlinear switching with very large on/off ratio, namely an increase of the output light by a factor of 10,000 for a 10% increase of the input light (published in *Applied Physics Letters* 110, 211104, 2017).

2. Ultra-low threshold for coherence. In work done in collaboration with the National Renewable Energy Lab in Golden, Colorado, the team demonstrated that the polariton coherent emission can be produced with extremely low pump intensity, namely a 0.57 mW continuous-wave pump into a defocused, 75 micron spot, an intensity orders of magnitude below all previous work. This was made possible both by the long lifetime of the polaritons and a strain-trapping method (published in *Optics Letters* 42, 1165, 2017).

3. Effect of a polariton condensate on electrical transport. The main topic of this project has been the interaction of electrical current with a polariton condensate. The Snoke group has successfully developed a method to electrically contact the quantum wells which run through the polariton condensate structures, and have shown that the presence of the condensate dramatically increases the electrical current (i.e., dramatically decreases the resistance), as shown in FIGURE 4. This work has been submitted to Physical Review Letters for publication, and is available as a preprint at arXiv:1710.10920. Theorist Alexey Kavokin has argued that this is evidence of exciton-mediated superconductivity, although it is too soon to confirm this. Theory led by co-PI Allan MacDonald, submitted to *Physical Review B* and is available at arXiv:1710.05826, has shown that in any case the coherent condensate is affected by current, which has been confirmed experimentally.

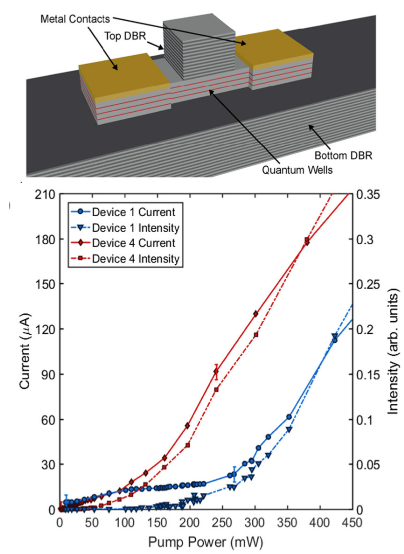

FIGURE 4

Current and light emission as a function of optical pump power at constant applied voltage, for two structures like that shown above, with different condensate thresholds.

D. Chiral Majorana Fermion Modes in a Quantum Anomalous Hall Insulator/Superconductor Structure

Professor Kang L. Wang, University of California - Los Angeles, MURI Award

The goal of this project is to realize the chiral Majorana fermion mode in a quantum anomalous Hall insulator (QAHI)/superconductor hybrid structure. In FY17, the research team integrated these two distinct classes of materials and for the first time experimentally demonstrated the quantized evidence of Majorana fermions.

The Majorana fermion is a hypothetical particle that is its own antiparticle. In 1937, Ettore Majorana proposed a particle being its antiparticle. This presence of Majorana has profound implications in cosmology, elementary particle physics and condensed matters. Thus since its inception, Majorana has been under intensive pursuit both theoretically and in experiments. Its non-Abelian braiding property can potentially be used to implement topological qubits in fault-tolerant quantum computers. In condensed-matter systems, theory predicted that Majorana fermions could be hosted in a superconductor, but superconductors do not have these properties, and the experiments to ascertain its presence is almost impossible. In this study, the team demonstrated the presence of Majorana fermions in chiral topological superconductor. A QAHI was interfaced with a superconductor (Nb) and resulted a chiral topological superconductor region due to the proximity effect sandwiched in between two QAH regions (SEE FIGURE 5). The team found that during a sweep of the external magnetic field, the edge transport configuration undergoes a transition. This first quantized signature gives the first firm evidence of the presence Majorana fermions in the QAHI-superconductor system, that in the long term could be engineered to serve as the building block for topological quantum computations.

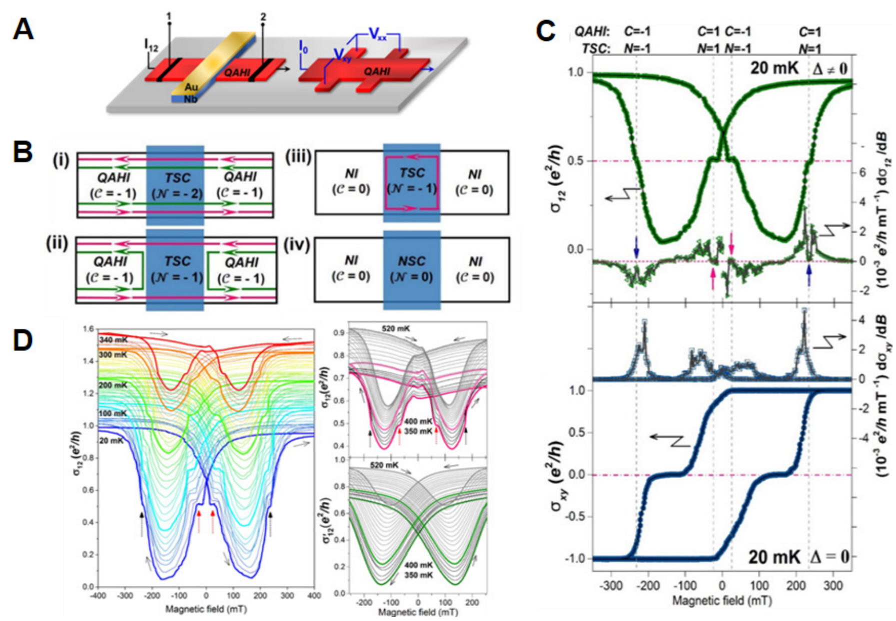

FIGURE 5

Observation of chiral Majorana edge mode in QAHI-superconductor heterostructure. (**A**) Schematic of a topological superconductor device consisting of a QAHI $(Cr_{0.12}Bi_{0.26}Sb_{0.62})_2Te_3$ thin film (6 nm thick) and a superconductor Nb bar. A QAHI Hall bar was also fabricated on the same wafer as a reference. (**B**) The edge transport configurations of the topological superconductor device during a sweep from saturation state (i) to insulating states (iii and iv). During the transition, a single chiral Majorana mode (ii) emerges. (**C**) σ_{12} as a function of external perpendicular magnetic field obtained from the device at 20 mK. When superconductivity is induced on the top surface of the QHAI, σ_{12} shows additional half-integer plateaus (~ 0.5 e^2/h) between the transitions of the QAHI C=±1 and the normal insulator and the derivative of σ_{12} with respect to the magnetic field. Topological transitions are marked by dashed lines and arrows. (**D**) Temp-dependent magneto-conductance in topological superconductor device and QAHI device. The half-plateau survives beyond 300 mK but indeed becomes less pronounced at higher temp due to the interference from trivial thermally activated bulk carriers.[1]

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[1] He L, Pan L, Stern AL, et. al. (2017). Chiral Majorana Fermion Modes in a Quantum Anomalous Hall Insulator-Superconductor Structure. *Science*. 357:294-299.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Mott transistor: Fundamental Studies and Device Operation Mechanisms

Investigator: Professor Shriram Ramanathan, Purdue University, Single Investigator Award
Recipient: U.S. Naval Research Laboratory (NRL)

The objective of this research was to investigate electronic transport mechanisms in strongly correlated semiconductors for possible applications in low power electronics. By controlling the occupancy of orbitals in a correlated perovskite semiconductor, it is possible to realize numerous electronic resistance states. This occurs by the means of engineering strong electron correlations in the material. In the research project, the oxide $SmNiO_3$ was investigated as a model system. By adding electron dopants such as hydrogen into the lattice using Pt or Pd electrodes, the PI and team were able to systematically vary the electron population in the nickel site orbitals. Upon half-filling condition, there is a strong Coulomb repulsion between electrons that hinders electronic conduction, leading the material to become an insulator (see FIGURE 6). By controlling the number of nickel sites affected by the dopant, it is therefore possible to control the overall resistance of the device. The device therefore exhibits electronic plasticity that can be exploited in neuromorphic learning and brain-like computation. The PI has fabricated two-terminal devices using $SmNiO_3$ with catalytic electrodes, which transitioned to the NRL Electronics branch for further studies, including electronic transport studies to induce various resistance states and understand their volatility. In the longer term, these measurements may inform the design of new semiconductors for neuromorphic intelligence.

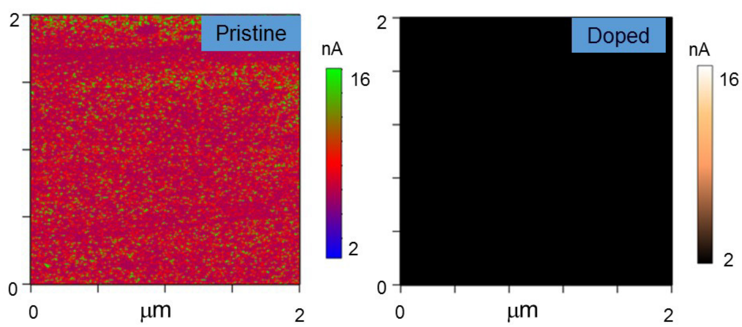

FIGURE 6

Conducting AFM image of pristine and doped $SmNiO_3$. (A) Scanning conducting force microscopy image of $SmNiO_3$ prior to doping. The color contrast indicates the material is conducting charge and the conduction is homogenous. (B) Conducting AFM map after the doping. The dark contrast indicates electronic transport is nearly fully suppressed due to charge localization. This massive suppression in conduction is due to added electrons anchoring to the Ni e_g orbitals. The extent of resistance change can be controlled carefully by varying the doping level creating unprecedented electronic plasticity that is of potential relevance to neuromorphic computing.

B. Terahertz Metasurfaces for Wavefront Control and Waveform Synthesis

Investigator: Professor Daniel Mittleman, Brown University, STIR and Single Investigator Awards
Recipient: Army Missile and Aviation Research Development and Engineering Center

The objective of this research is to develop a metasurface with adaptive and controllable meta-elements which will shape and direct THz radiation. The metasurface acts as a leaky wave antenna, radiating from THz surface waves at an angle determined by the specific frequency of the THz waves. The angle of radiation, the shape of the wavefront, the frequency and phase content of the THz radiation is controlled by adjusting the individual elements of the meta-surface. In the first experiments, the surface waves are exited at the edge of the metasurface by a broadband THz signal and radiate from the surface (see FIGURE 7). In this initial experiment, the meta-surface was modulated in 1 dimension, with results demonstrating the feasibility of modulating the frequency content of the surface waves using the meta-surface and demonstrate the understanding of the phenomena with the close match of simulation and experiment (see FIGURE 8). In a practical THz antenna the meta-surface could be modulated in 2 dimensions for a more complex wavefront. Experimental results have been made by Brown University graduate students working with researchers at AMRDEC. A practical THz waveshaping antenna will be pursued by AMRDEC in conjunction with Brown University researchers.

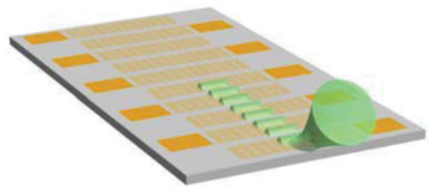

FIGURE 7

THz surface waves excited at edge of meta-surface and radiating into space. The meta-surface elements are controlled individually to shape the frequency content of the surface waves.

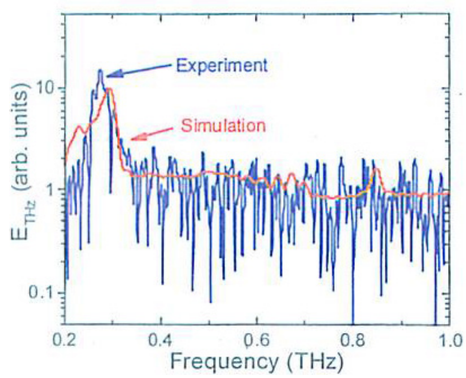

FIGURE 8

THz surface waves transmitted through the adaptive meta-surface.

C. Coupling of Grating-Confined Zig-zag Modes for High Power, Brightness Laser Diodes

Investigator: Professor Lin Zhu, Clemson U., Single Investigator Award
Recipient: DoD Directed Energy Joint Technology Office

Prof. Lin Zhu has investigated new routes to increased brightness diode lasers in a recent YIP (Young Investigator Program) program. His work resulted in zig-zag patterned, 100 micron wide waveguide lasers with multiple output ports. Coherently coupled output ports were demonstrated with power levels around 1 W. However, the work failed to progress further in a follow-on STIR project due to limited resources hindering progress on embedded, sub-surface gratings requiring epitaxial regrowth. Regrowth processes can be time consuming and require substantial effort to optimize. These results transitioned to receive follow-on investment by the DoD Directed Energy Joint Technology Office, a more substantial $2.25M program has begun. As a result of initial funding of the ARO YIP and STIR programs, the PI is starting a program with the Professor Ganesh Balakrishnan (Univ. of New Mexico), and Dr. Jonah Jacob of the Science Research Laboratory, to explore the potential of the lasers. By burying the gratings below the surface and regrowing the top conductive layers, a more substantial coupling can occur between the laser's optical mode and the grating allowing one to make a much smaller grating. Such designs will not inhibit current flow so that the expectation for power output is at 10 W per stripe. Combining multiple zig-zags of the pattern, as already demonstrated with the surface gratings, one can envision scaling of the lasers up to several orders of magnitude beyond this creating powerful new capabilities for the military. Particular interest in their use could be for pumping fiber lasers with much higher brightness and efficiency as well as direct diode propagation applications.

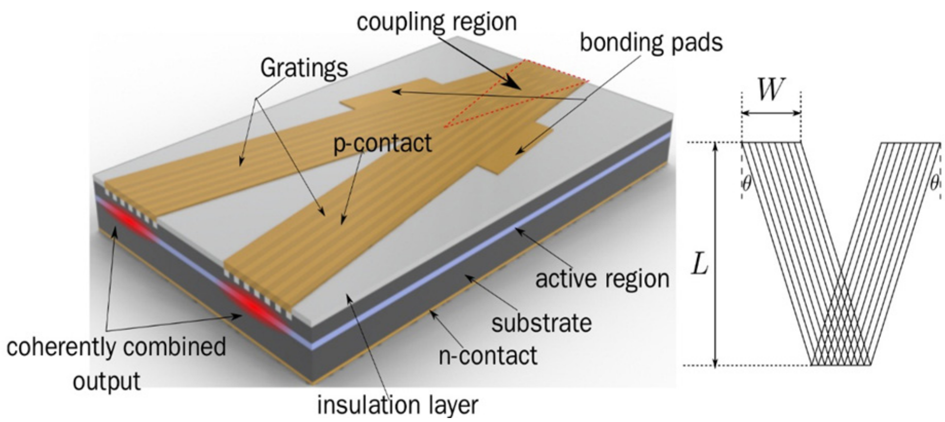

FIGURE 9

Schematic plot of coherently combined angled-grating broad-area laser. The V-shape is one part of a zig-zag laser architecture that would be fully integrated, scalable and require no external components to achieve coherent combining

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Triggerable Molecular Devices for the Real-time, Simultaneous, Nano-scale Detection and Modulation of Intracellular Bio-electric Fields

Professor Andrea Armani, University of Southern California, Single Investigator Award

The purpose of this research is to invent and demonstrate a unique molecule which functions with independent control to modulate the electric field local to the molecular device and to detect the local bioelectric field in the intracellular region and to use the device to explore the role of voltage dependent calcium ion channels on cellular functions. The molecular device concept consists of a modulator molecule and a detector molecule covalently bonded using click chemistry (see FIGURE 10). The two constituents form nano-scale device that can simultaneously modulate and detect the bioelectric intracellular fields with nano-scale spatial resolution. Visible light modulates the resistance of the modulator side of the device, modulating the local E field near the device. Near IR light stimulates a chromophore in the detector side of the device, which emits in the visible, with the magnitude of the emission proportional to the magnitude of the local bio-electric field.

It is anticipated that in FY18, Professor Armani will synthesize and characterize the covalently bonded molecular device and demonstrate the operation in the cell wall membrane. Subsequent research will optimize the device and resolve issues of insertion into the intracellular region.

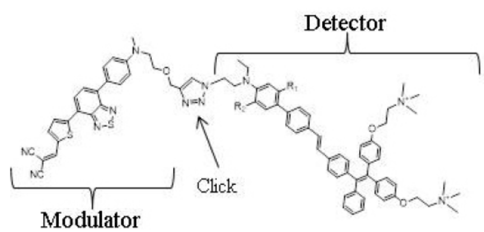

FIGURE 10

Proposed molecular device for real-time modulation and reporting of bioelectric fields. The modulator molecule and the detector molecule are covalently joined by click chemistry.

B. Hydrodynamic Electron Transport in 2D Materials for Nanoelectronics

Professors Philip Kim (PI) and Donhee Ham (co-PI), Harvard University; Dr. Kin Chung Fong (co-PI), BBN Raytheon, Single Investigator Award

The goal of this research is to study and utilize the hydrodynamic electron transport in 2D materials for novel RF and THz electronic device applications. It is anticipated that in FY18, the research team will study the kinetic inductance of graphene in the hydrodynamic plasmon transport regime. The large kinetic inductance LK of graphene allows its plasmons (charge density oscillations) to have very small propagation velocities (of ~c/100). Such plasmons have been measured in the microwave and far-infrared regimes, and this experiment seeks to bridge the frequency gap by making a direct measurement of the graphene plasmons propagation constant. The proposed experiment is enabled by 2 key features that combine to enable the quality factor $Q = \omega LK/R$ of the plasmon oscillations to be greater than 1. Firstly, Virginia Diode VNA extenders allow the team to make vector network measurements of the graphene devices at 330GHz and at room temperature. Secondly, the very large mobility of graphene (~100 000 cm^2 / Vs) encapsulated in hBN resulting in much lower device resistances leads to relatively low plasmon losses even at room temperature. Preliminary measurements of the graphene plasmon velocity have been made, demonstrating the gate dependence of the graphene plasmon velocity (see FIGURE 11). In addition, the team anticipates further tuning the gate velocity by injecting current, applying a drift velocity to the electrons that are carrying the plasmon. The drift velocity is predicted to manifest itself as a nonreciprocal plasmon transmission, with differing forward and backward propagation velocities.

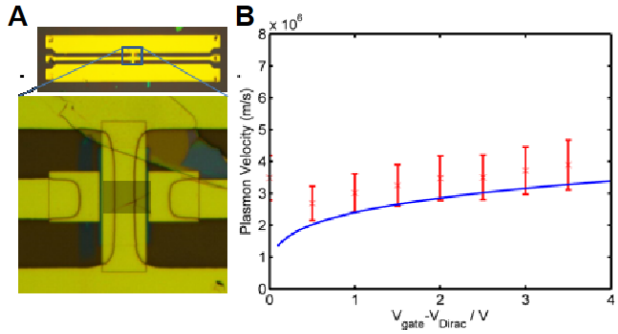

FIGURE 11

Graphene Kinetic Inductance Device and Gate Dependent Plasmon Velocity. (**A**) Optical Image of device showing the coplanar waveguides used to couple mm-waves into the hBN-encapsulated graphene (grey region, graphene not visible under top-gate). (**B**) Extracted plasmon velocities. The blue line is the theoretical lossless plasmon velocity.

It is also anticipated that in FY18 the research team will study the electronic hydrodynamics by investigating its difference from the conventional ohmic flow. Specifically, the team will measure the electron temperatures at different part of the graphene device and look for the heat flow pattern due to convective heat conduction. In the ohmic flow, the Joule heating can dissipate out of the graphene electrons by diffusing to the side and sinking into the electrical terminals, which act as a thermal reservoir (see FIGURE 12). The temperature profile is symmetric regardless of the charge flow direction. In contrast, heat can be conducted by the convective term, $v \cdot \nabla v$, in the Navier-Stokes Equation in the hydrodynamic flow, where $\boldsymbol{v}$ is the velocity of the hydrodynamic fluid. This convective term can generate a temperature difference that depends on the direction of the current. The comparison of the diffusive and convective heat flows in connection with the charge flows will interrogate the hydrodynamic behaviors of the graphene electrons.

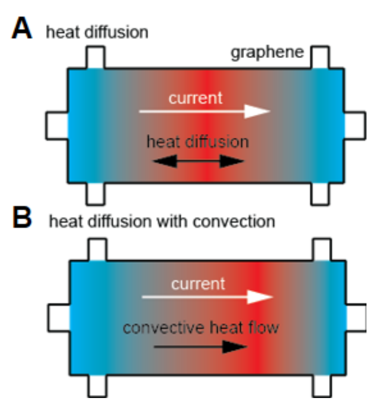

FIGURE 12

Convective heat flow measurement scheme. When the electronic diffusion dominates the dissipation of Joule heating out of the graphene sample via the metallic contacts, the temperature profile is symmetric (**A**) with respect to the direction of the applied bias current in the case of ohmic flow. (**B**) The hydrodynamic can modify the heat transport with the convection breaks the symmetry in temperature profile.

C. Negative Curvature Anti-Resonant Hollow Core Optical Fibers

Professor Rodrigo Amezcua-Correa, University of Central Florida, Single Investigator Award

This research will study and demonstrate novel air guiding fibers that address critical physical limitations of optical fibers. These radically new anti-resonant hollow core fiber (HCF) designs have the potential for light transport in a single mode over wide transmission windows with ultra-low loss (<1 dB/km) and orders of magnitude higher damage and nonlinear thresholds compared to conventional fibers (see FIGURE 13). Fibers with this level of performance can open up applications not possible using current fibers such as: long distance high optical power transport (kW power delivery over km range), extreme peak power/energy delivery, low latency broadband data transmission, as well as low-loss UV and mid-IR transmission. Such advantages are possible due to the hollow core guiding region that is free of nonlinearities caused by typically glass-based gain media. In the future work, the ability to implement significantly better anti-resonant designs is anticipated. Low losses well below dB/km level and spectral transmission bandwidths over very wide regions could open new applications hardly imaginable. Ideas could be thought of in terms of garnering such a broad spectrum at one end of the fiber to transmit perfectly kilometers away. Particular applications can be seen for spectral sensing, imaging, and much broader-band communications than previously imagined. Quantum communications with entangled properties could be enhanced and would not require quantum frequency conversion because of the potentially low loss down into the UV. Other applications in the UV spectrum may come to light since this region has not been useful due to much higher transmission losses caused by the air below 200 nm. Vacuum pumping such hollow fibers though may enable long distance transmission of very high photon energy signals.

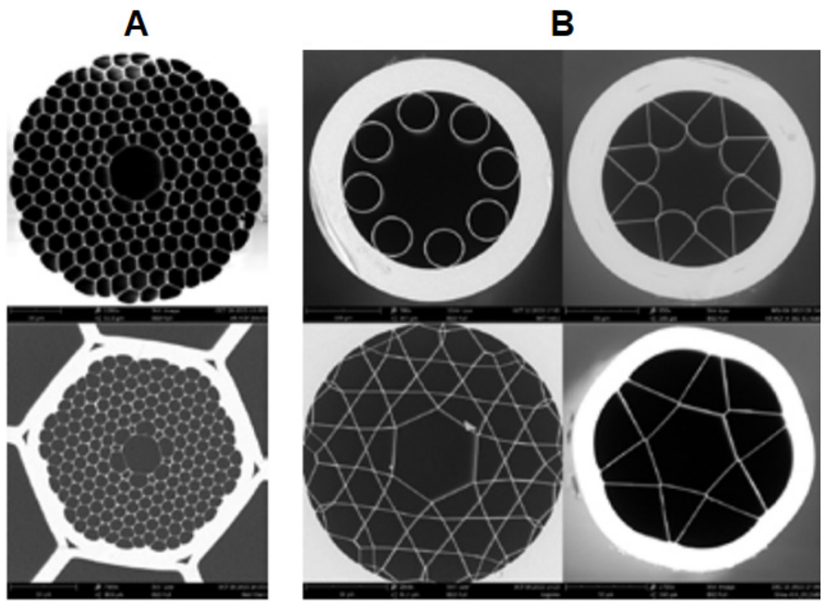

FIGURE 13

Scanning electron microscope (SEM) image of HCF. (A) Hollow core PBG fibers and (B) antiresonant HCFs – central column antiresonant HCF with non-touching capillaries and kagome fiber. Right column negative curvature antiresonant fiber and hexagram fiber.

VI. DIVISION AND DIRECTORATE STAFF

A. Division Scientists

Dr. David Stepp
Division Chief (Acting)

Dr. Michael Gerhold
Program Manager, Optoelectronics
Program Manager (Acting), Electronic Sensing

Dr. James Harvey
Program Manager (Acting), Electromagnetics and Radio-frequency Electronics

Dr. Joe Qiu
Program Manager (Acting), Nano- and Bio-Electronics

B. Directorate Staff and Contract Support

Dr. David Stepp
Director, Engineering Sciences Directorate

Ms. Liza Wilder
Administrative Specialist

Mr. George Stavrakakis
Contract Support

Ms. Megan Hammond
Contract Support

CHAPTER 6: LIFE SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2017* is to provide an annual historical record summarizing the programs and basic research supported by ARO in FY17. ARO's mission is to support creative basic research resulting in new science that enables new materials, devices, processes, and capabilities for the current and future Soldier. This chapter provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions enabled by the ARO Life Sciences Division in FY17.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Life Sciences Division supports research to discover and control the properties, principles, and mechanisms governing DNA, RNA, proteins, organelles, molecular and genetic systems, prokaryotic cells, eukaryotic cells, unicellular organisms, multicellular organisms, multi-species communities, individual humans, and groups of humans. More specifically, the Division aims to promote basic research to elucidate the fundamental physiology underlying perception, cognition, neuro-motor output and non-invasive methods of monitoring cognitive states and processes during normal activity; basic research to understand antimicrobial resistance mechanisms; microbial community interactions including biofilm formation, cell-to-cell communications, population dynamics and host-pathogen/symbiont interactions; studies of organisms that are not culturable; studies of organisms at the single cell or mixed population (*e.g.*, metagenomic) level; studies of organisms that have adapted to grow or survive in extreme environments; identification and characterization of gene function, gene regulation, genetic interactions, gene pathways, gene expression patterns, mitochondrial regulation and biogenesis, nuclear and mitochondrial DNA replication, mutagenesis, oxidative stress, DNA repair, and regeneration; studies in structural biology, protein and nucleic acid structure-function relationships, molecular recognition, signal transduction, cell-cell communication, enzymology, cellular metabolism, and synthetic biology; and research to understand human behavior across different temporal, spatial and social scales. The results of this research will lay a foundation for future scientific breakthroughs and will enable new technologies and opportunities to modernize and maintain the technological and military superiority of the U.S. Army.

2. Potential Applications. Research managed by the Life Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the discoveries uncovered by ARO in the life sciences may provide new technologies for protecting the Soldier, for optimizing warfighter mental and physical performance capabilities, for creating new biomaterials, for advances in synthetic biology for energy production, intelligence, and bioengineering, and for new capabilities for predicting group behavior and change.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Life Sciences Division coordinates and leverages research within its Program Areas with many other agencies, including the Defense Threat Reduction Agency (DTRA), the Defense Advanced Research Projects Agency (DARPA), the Army Natick Soldier Research Development and Engineering Center (NSRDEC), the U.S. Army Corps of Engineers (USACE), the Army Research Institute (ARI), the Army Medical Research and Materiel Command (MRMC), the National Institutes of Health (NIH), the Intelligence Advanced Research Projects Agency (IARPA), the Department of Homeland Security (DHS), the Army Criminal Investigation Laboratory (ACIL), the Federal Bureau of Investigation (FBI), the Office of Naval Research (ONR), and the Air Force Office of Scientific Research (AFOSR). In addition, the Division frequently coordinates with other ARO and ARL Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches.

For example, interactions with the ARO Chemical Sciences Division include promoting research to understand abiotic/biotic interfaces. The Life Sciences Division coordinates its research portfolio with the Materials Science Division to pursue the design and development of new biomaterials. The Life Sciences Division also coordinates extensively with the Mathematical Sciences Division to develop new programs in bioforensics and microbiomes, and with the Materials Science and the Mechanical Sciences Divisions to understand the effects of blast on synapses. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

The Division's research portfolio will also reveal previously unexplored avenues for new Army capabilities while also providing results to support the ARL ERAs of (i) Intelligent Teams, (ii) Impact of Operating in a Contested Environment, and (iii) Implementation. In addition, the Division supports the (i) the Human Sciences Campaign's goals to discover and predict human cognitive, physical, and social behaviors, as well as the role of training paradigms in building expertise, and to characterize the fundamental aspects of social network dynamics involving ethics, values, trust, social-cultural, economic, and geopolitical effects, (ii) the Assessment and Analysis Campaign's goal to identify human capabilities and limitations, (iii) the Information Sciences Campaign's goal to develop predictive models that consider the availability of power or food sources and the potential for social unrest or insurgency activity, (iv) the Sciences for Lethality-and-Protection Campaign's goal to predict and exploit interactions between information and humans, including the impact of trust and value on negotiation, and (v) the Materials Research Campaign's goal to exploit the evolutionary solutions created by nature and create similar structures using synthetic biology.

B. Program Areas

The Life Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY17, the Division managed research within these seven Program Areas: (i) Genetics, (ii) Neurophysiology of Cognition, (iii) Biochemistry, (iv) Microbiology, (v) Social and Behavioral Science, and the International Programs (vi) Human Dimension and (vii) Synthetic Biology. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Genetics. The scientific goals of this Program Area are to identify and characterize the mechanisms and factors that influence DNA stability and mutagenesis, gene expression, and genetic regulatory pathways in prokaryotes, eukaryotes, and eukaryotic organelles. This program also seeks to understand genetic instability at a population level. The program supports basic research on mitochondrial regulation and biogenesis, oxidative phosphorylation, oxidative stress, and the interactions and communication between the mitochondria and the nucleus. The Genetics Program also supports basic research to develop an empirical understanding of general mechanisms by which genomic, transcriptomic, and proteomic components respond to alterations in the population-genetic environment. A third area of emphasis is the identification, characterization, and modulation of genetic pathways and molecular cascades that determine the responses to stress and trauma. A final area of emphasis is to create the genetic foundation to be able to extract provenance information from both prokaryotic and eukaryotic DNA.

This Program Area supports high-risk, high payoff basic research that has the potential to create new Army capabilities, to optimize warfighter mental and physical performance capabilities, to reduce the effect of PTSD, stress, and pathogens on warfighter readiness and Army capabilities, and to develop new sources of intelligence.

2. Neurophysiology of Cognition. The objective of this Program Area is to support non-medically oriented research to elucidate the fundamental physiology underlying perception, sensorimotor integration and cognition. Examples of research areas under this program can include the psycho-physiological implications of brain-machine interfaces that optimize auditory, visual and/or somatosensory function; display and control systems based on physiological or psychological states; measuring and modeling individual cognitive dynamics and decision making during real-world activity and uncovering the cellular biology of neuronal function.

This Program Area is divided into two major research thrusts: (i) Multisensory Synthesis and (ii) Neuronal Computation. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goals. Research in the Multisensory Synthesis Thrust aims to understand how the human brain functions in relation to the interaction of multisensory, cognitive and motor processes during the performance of real-world tasks. Basic research focused on mapping, quantifying and modeling distributed neural processes that mediate these features are being used to develop better understanding of the underlying bases of cognitive processes for eventual application to Soldier performance enhancement and improved human-machine symbiosis. Research in the Neuronal Computation Thrust is focused on understanding how living neuronal circuits generate desirable computations, affect how information is represented, show robustness to damage, incorporate learning and facilitate evolutionary change. Cell culture, brain slice and in vivo models are being used to develop better understanding of living neural networks for eventual application in Army systems that might include novel direct neural interfaces.

While these research efforts focus on high-risk, high pay-off concepts and potential long-term applications, current research may ultimately enable the development of neural biofeedback mechanisms to sharpen and differentiate brain states for possible direct brain-machine communication, identifying individual cognitive differences and new training paradigms for improved Soldier performance.

3. Biochemistry. The goal of this Program Area is to elucidate the mechanisms and forces underlying the function and structure of biological molecules. This research may enable the design and development of novel materials, molecular sensors and nanoscale machines that exploit the exceptional capabilities of biomolecules.

This Program Area supports two research Thrusts: (i) Biomolecular Specificity and Regulation (BSR), and (ii) Biomolecular Assembly and Organization (BAO). Within these Thrusts, innovative research efforts are identified and supported in pursuit of the vision of this program. Efforts in the BSR Thrust aim to identify the determinants of the specificity of molecular recognition and molecular activation/inactivation to modulate and control specificity and activity through protein engineering and synthetic biology approaches. Research in the BAO thrust aims to explore the fundamental principles governing biological self-assembly, to understand and control the relationships between molecular structure and biological materials, and to identify innovative approaches to support biological activity outside of the cellular environment.

Research supported by this program promotes potential long-term applications for the Army that include biosensing platforms that incorporate the exquisite specificity of biomolecular recognition, nanoscale biomechanical devices powered by motor proteins, novel biotic/abiotic materials endowed with the unique functionality of biomolecules, drug delivery systems targeted by the activity and specificity of biomolecules, electronic and optical templates patterned at the nanoscale through biomolecular self-assembly, and novel power and energy systems that utilize biomolecular reaction cascades.

4. Microbiology. This Program Area supports basic research in fundamental microbiology. There are two primary research thrusts within this program: (i) Microbial Survival Mechanisms and (ii) Analysis and Engineering of Microbial Communities. The Microbial Survival Mechanisms thrust focuses on the study of the cellular and genetic mechanisms and responses that underlie microbial survival in the face of environmental stress. These stressors include extremes in temperature, pH, or salinity; the presence of toxins including metals and toxic organic molecules; oxidative stress; and cellular starvation and the depletion of specific nutrients. Research approaches include fundamental studies of microbial physiology and metabolism, cell biology, and molecular genetics that examine key cellular networks linked to survival, microbial cell membrane structure and the dissection of relevant critical signal transduction pathways and other sense-and-respond mechanisms. The Analysis and Engineering of Microbial Communities thrust supports basic research that addresses the fundamental principles that drive the formation, proliferation, sustenance and robustness of microbial communities through reductionist, systems-level, ecological and evolutionary approaches. Bottom-up analysis of information exchange, signaling interactions and structure-function relationships for single and multi-species communities within the context of planktonic and biofilm architectures is considered. Of joint interest with the ARO Biomathematics Program, research efforts that advance our ability to work with complex biological data sets to increase understanding of microbiological systems marked by ever-increasing complexity are considered.

While these research efforts focus on high-risk concepts, research supported by this program promotes a range of long-term applications for the Army, including strategies for detecting and classifying microbes, for controlling bacterial infections, for harnessing microbes to produce novel materials, to protect materiel, and/or to efficiently produce desirable commodities. In addition, understanding how microbes adapt is crucial for advancing studies in other fields, including genetics, environmental science, materials science, and medicine.

5. Social and Behavioral Science. The goal of this Program Area is to gain a better theoretical understanding of human behavior at all levels, from individuals to whole societies, for all temporal and spatial scales, capturing interdependencies of social, natural, and physical systems through the development of mathematical, computational, simulation and other models that provide fundamental insights into factors contributing to human socio-cultural dynamics and societal outcomes (see FIGURE 1).

This Program Area is divided into two research Thrusts: (i) Sensing and Modeling Human Social Behavior, and (ii) Interdependencies across Social, Natural, and Physical. The program supports research that focuses on the theoretical foundations of human behavior at various levels (individual actors to whole societies) and across various temporal and spatial scales. This includes, but is not limited to, research on the evolution and dynamics of social systems and organizations, human adaptation and response to both natural and human induced perturbations (*e.g.*, environmental evolution, mass migration, war, attempts at democratization, movements for social justice), introduction of new technologies (including autonomous systems and artificial intelligence), interactions among humans, natural systems, and physical systems, alongside the role of culture and cognition in accounting for variations in human behavior, human decision-making under risk and uncertainty, the search for organizing principles in social systems, and the emergent and latent properties of dynamic social systems and networks. The research involves a wide range of approaches, including computational modeling, mathematical modeling, agent-based simulations, econometric modeling and statistical modeling, comparative-historical analyses, to name a few. The program also recognizes the fact that the building and validation of models in the social sciences is often limited by the availability of adequate and appropriate sources of primary data. A component of supported research includes the collection of primary data for model development and testing. The program also supports research to develop methodologies (*e.g.*, measurement, data collection, statistical methods, and research designs) that may provide an improved scientific understanding of human behavior.

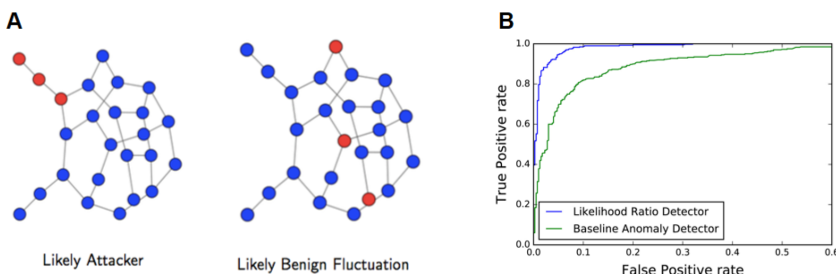

FIGURE 1

Examples of studies to measure and uncover factors contributing to human socio-cultural dynamics. (**A**) Detecting legitimate vs. false attacks on a social system depends on structural location and dynamics of potential attack agents, independent of social structure, which is consistent across the two figures. (**B**) Reduction of false positives (i.e., erroneous detection of attacks) through development of new likelihood ratio detector modeling based on social science research on embeddedness of attacking agents. This research offers new ways to detect risk and avoid misallocation of resources toward defense against benign threats to improve operational efficiencies and focus resource allocations on legitimate attacks.[1]

Research focuses on high-risk approaches involving highly complex scientific problems in the social sciences. Despite these risks, the research has the potential to make significant contributions to the Army through applications that will, for example, improve decision-making at various levels (policy, combat operations), create real-time computer based cultural situational awareness systems for tactical decision-making, increase the predictability of adversarial and allied intent, and produce integrated data and modeling in situ for rapid socio-cultural assessment in conflict zones and in humanitarian efforts.

6. Human Dimension (International Program). As one of the ARO International Programs, the Human Dimension Program supports multidisciplinary research and facilitates engagement of RDECOM scientists with international researchers to identify and model the co-evolutionary multiscale dynamics of human neural, cognitive, physical, and social systems, and to exploit and leverage significant scientific advances in other countries. The Program Area supports multidisciplinary basic research and identifies top researchers in areas

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[1] Grana J, Wolpert D, Neil J, Xie D, Bhattacharya T, Bent R. (2016). A likelihood ratio anomaly detector for identifying within-perimeter computer network attacks. *J. Netw. Comput. Appl.* 66:166-179.

that include neural and cognitive sciences, behavioral sciences, human factors, and neural engineering with an emphasis on modeling, predicting and enhancing human perceptual, cognitive, affective, physical, and social performance. An overarching goal of the program is to uncover the neural, biophysiological and cognitive mechanisms underlying individual, group and societal cognition and performance across multiple time scales.

This Program Area is divided into two major focus areas: (i) Cognitive-Physical Interactions and (ii) Cognitive-Social Interactions. Within these focus areas, researchers and high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goals. Research in the Cognitive-Physical Interactions focus areas seeks to use multimodal approaches to uncover dynamic and multiscale interactions of neural-cognitive and physiological systems. The goal is to advance experimental and analytical tools to develop comprehensive understanding of human performance as it relates to individual state-trait variability on human performance, human-system integration and team intelligence. Research in the Cognitive-Social Interactions area seeks to develop new theories to understand the dynamic interrelationships between individual cognition, decision-making and the role that these influences dynamically play on interactions with large and small social systems. Multidisciplinary opportunities are sought to advance the analytical and experimental tools required to describe the underlying mechanistic interactions as they co-evolve in time and space.

In the long term, research in the human dimension may enable new training tools to predict and optimize cognitive/physical performance and team intelligence, interfaces enabling humans to more efficiently control machines and multiscale predictive models of complex individual – societal dynamics.

7. Synthetic Biology (International Program). The International Synthetic Biology Program Area supports research to develop new synthetic biology techniques to understand basic biology and to design biological systems and processes with high reliability, scalability, and predictability, to create new Army capabilities

The Program's thrusts investigate the ways in which biological systems can be made robust, complex, and adaptive. Such biosystems may synthesize biomaterials or high-grade biochemicals, provide sensors, or interface with abiotic systems. Naturally occurring processes may be combined with techniques that do not occur in nature, such as gene shuffling and directed editing, to create organisms that are both engineered and adapted. The program also focuses on the creation and maintenance of hybrid prokaryotic-eukaryotic symbiotic systems. Such systems can potentially combine the relative ease of engineering of prokaryotes with the robustness and processing capability of eukaryotes. Studies of the innate immune system of both plants and animals are also of interest, as well as intracellular immune processes.

Pursuing these high-risk avenues for synthetic biosystems is essential to provide the Army with game-changing advances: extraordinary biomaterials that are lightweight, self-healing, and rugged; the ability to use photosynthetic extraction of energy and carbon to reduce logistic needs; probiotics and nutritional support; hardened sensors and displays of superior sensitivity; and energy production in austere environments.

C. Research Investment

The total funds managed by the ARO Life Sciences Division for FY17 were $97.5 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY17 ARO Core (BH57) program funding allotment for this Division was $9.3 million and $2.1 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $7.4 million to projects managed by the Division. The Division also managed $60.2 million of Defense Advanced Research Projects Agency (DARPA) programs, $2.7 million for Minerva Research Initiative projects, and $4.2 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.9 million for contracts. The Army's Institute for Collaborative Biotechnologies received $7.7 million. In addition, $2.4 million was provided for awards in the Historically Black Colleges and Universities and Minority Serving Institutions (HBCU/MSI) Programs, including funding for DoD-funded Partnership in Research Transition (PIRT), DoD-funded Research and Educational Program (REP) projects, and $0.4 million of the Division's ARO Core (BH57) funds, with the latter included in the BH57 subtotal above.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY17 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY17 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY17, the Division awarded 23 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Joshua Banta, The University of Texas - Tyler; *The Metabolism and Genomics of Industrial Vs. Wild Strains of Clostridium Acetobutylicum*
- Professor Elisa Bienenstock, Arizona State University; *Identifying Key Actors in Heterogeneous Networks*
- Professor Berry Brosi, Emory University; *Quantitative Metabarcoding of Pollen for Security-Related Forensics*
- Professor James Culver, University of Maryland - College Park; *Nano- and Micro-scale Patterning of Virus Assembled Enzymatic Cascades for Bio-Energy Harvesting*
- Professor Bernie Daigle, University of Memphis; *Knowledge-Assisted Multi-omic Biomarker Identification for Posttraumatic Stress Disorder*
- Professor Simon DeDeo, Carnegie Mellon University; T*he Role of Information in Structured Conflict*
- Professor Helen Irving, Monash University (Australia); *Controlling A Novel Catalytic Center Within An Innate Immune System Protein To Dampen Or Heighten The Immune Response*
- Professor Sarah Jones, Monash University (Australia); *Immunospheres: Creating An Immune System In A Microparticle*
- Professor William Kalkhoff, Kent State University; *Team Perception and Performance Under Threat*
- Professor David Kaplan, Tufts University; *Dynamic Materials Based On Bioengineered Fibrous Proteins*
- Professor Andy Liwang, University of California - Merced; *Birth of the Metamorphome*
- Professor Derek Lovley, University of Massachusetts - Amherst; *Mechanisms for Electrical Communication in Methane-Producing Microbial Communities*
- Professor Martin McCullagh, Colorado State University - Ft. Collins; *Molecular Driving Forces of Peptide-Based Biomaterials*
- Professor Daniel Morse, University of California - Santa Barbara; *A Switch Controlling Biomolecular Reconfigurability*

- Professor Hannes Neuweiler, University of Wuerzburg (Germany); *Investigation Of The Molecular Architecture Of Spider Silk Protein Assembly Using High-Resolution Fluorescence Microscopy*
- Professor Dianne Newman, California Institute of Technology; *Phenazine-Mediated Extracellular Electron Transfer And Microbial Community Organization*
- Professor Peter Peregrine, Human Relations Area Files, Inc.; *Social Resilience to Nuclear Winter: An Analysis of the A.D. 536 Atmospheric Event*
- Professor Srivatsan Raman, University of Wisconsin - Madison; *Radical Redesign Of An Allosteric Biosensor To Respond To New Ligands*
- Professor Dawn Robinson, University of Georgia Research Foundation, Inc.; *Measures of Emotion*
- Professor Luis Serrano, Fundacio Centre de Regulacio Genomica (Spain); *Genome Engineering Escherichia Coli To Enable Hybrid Prokaryotic-Eukaryotic Systems.*
- Professor William Swann, University of Texas - Austin; *Identity Fusion and Extreme Group Behavior*
- Professor Joe Tsien, Medical College of Georgia; *A Novel Approach to Predicting Resilience to Post-Traumatic Stress Disorder*
- Professor Ilana Witten, Princeton University; *Prefrontal Cortical Circuitry that Supports Learning in a Complex and Dynamic Environment*

2. Short Term Innovative Research (STIR) Program. In FY17, the Division awarded two new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Gerald Griffin, Hope College; *Effect of HSV-1 Latent Infection On Laser-Induced Axotomy*
- Professor Eleftherios Papoutsakis, University of Delaware; *Probing Novel Syntrophic Microbial Interactions*

3. Young Investigator Program (YIP). In FY17, the Division awarded one new YIP projects to drive fundamental research in areas relevant to the current and future Army. The following PI and corresponding organization received the new-start YIP award.

- Professor Joseph Dippong, University of North Carolina - Charlotte; *Vocal Accommodation Within Nonverbal Frequencies as a Marker of Status, Dominance, and Prestige*

4. Conferences, Workshops, and Symposia Support Program. The Division provided funds in support of a range of scientific conferences, workshops, and symposia that were held in FY17. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences, with the goal of supporting scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army, and to define the research needs, thrusts, opportunities, and innovation crucial to the future Army. Proposals requesting funding support, typically for less than $10K, were received and evaluated in line with the publicly available ARO BAA. In FY17, seven proposals were selected for funding by the Division to support FY17 conferences, workshops, or symposia.

5. Special Programs. In FY17, the Division also awarded five new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school and undergraduate students. These efforts were funded through the ARO Core Program and Youth Sciences Programs, for research to be performed at academic laboratories currently supported through active SI awards (refer to CHAPTER 2, Section IX).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Translating Biochemical Pathways to Non-Cellular Environment. This MURI began in FY12 and was awarded to a team led by Professor Hao Yan at Arizona State University. This MURI is exploring how biochemical pathways could potentially function in a non-cellular environment.

Cells provide a precisely organized environment to promote maximum efficiency of biochemical reaction pathways, with individual enzymatic components organized via multisubunit complexes, targeted localization in membranes, or specific interactions with scaffold proteins. The eventual translation of these complex pathways to engineered systems will require the ability to control and organize the individual components outside of the natural cellular environment. Although biological molecules have been successfully attached to inorganic materials, this process often requires chemical modification of the molecule and can restrict its conformational freedom. An alternative approach to maintain biological activity outside of the cell, while preserving conformational freedom, is to encapsulate enzymes within specialized materials or structures. Unfortunately, surface patterning of current encapsulating agents has not achieved the precision required to replicate the organizational capabilities of the cell.

The objective of this research is to develop the scientific foundations needed to design, assemble, and analyze biochemical pathways translated to a non-cellular environment using 3D DNA nanostructures. The MURI team is using DNA nanostructures to direct the assembly of selected biochemical pathways in non-cellular environments. The focus of this research is to develop the scientific foundations needed to translate multi-enzyme biochemical reaction pathways from the cellular environment to non-biological materials. The ability to translate biochemical reaction pathways to non-cellular environments is critical for the successful implementation of these pathways in DoD-relevant technologies including responsive material systems, solar cells, sensor technologies, and biomanufacturing processes.

2. Evolution of Cultural Norms and Dynamics of Socio-Political Change. This MURI began in FY12 and was awarded to a team led by Professor Ali Jadbabaie at the University of Pennsylvania. This MURI is exploring the cultural and behavioral effects on societal stability.

Recent events involving the diffusion of socio-political change across a broad range of North African and Middle Eastern countries emphasize the critically important role of social, economic and cultural forces that ultimately affect the evolution of socio-political processes and outcomes. These examples clearly demonstrate that radically different outcomes and chances for conditions of state stability result from the different institutional frameworks within these countries. It is well established in the social sciences that change in or evolution of institutions depends on the behavior patterns or culture of the people involved in them, while these behavior patterns depend in part on the institutional framework in which they are embedded. This dynamic interdependence of culture and institutional change means that the modeling of societal stability requires the coupling of individual modeling approaches describing such issues as trust and cooperation with models describing institutional dynamics.

The objective of this MURI is to develop fundamental theoretical and modeling approaches to describe the complex interrelation of culture and institutions as they affect societal stability. The research team is extending the cultural approaches from application to individuals, families, and villages, to address stability of the larger social group. The models developed in this MURI may ultimately provide guidance in data collection and analysis of data on local populations that can provide planners with models to anticipate the second or third-order ramifications of actions that impact local populations.

3. Simultaneous Multi-synaptic Imaging of the Interneuron. This MURI began in FY12 and was awarded to a team led by Professor Rafael Yuste at Columbia University. The research team is exploring how individual neurons act as computational elements.

Interneurons are highly networked cells with multiple inputs and outputs. It has been to date impossible to record all the inputs and outputs from even a single living interneuron with synaptic levels of resolution in a living brain. While there is information on the morphological, physiological, and molecular properties of interneurons as a class and on their general synaptic connections, there is still little direct information on the functional roles of individual interneurons in cortical computations, and especially not on how each synapse relates to all the others within a single cell. Coupled with tagging via fluorescent molecules and/or chromophores and genomic modifications to control co-expression, electro-optical imaging may provide a solution, due to its ability to achieve subwavelength resolution across a relatively wide field of view.

The objective of this research is to explain and quantitatively model the entire set of neurotransmitter flows across each and every individual synapse in a single living interneuron, with experimental preparations ranging from cell culture systems through model neural systems. The research team will use genetically-engineered mice expressing specific labels in specific interneurons, high-throughput electron microscopy, and super-resolution imaging techniques to reveal the connectivity and the location of the synapses. This research may ultimately provide models that predict the information transitions and transformations that underlie cognition at the smallest scale where such activity could take place. These models could revolutionize the understanding of how human brains instantiate thought, and may lead to applications such as neural prostheses.

4. Artificial Cells for Novel Synthetic Biology Chassis. This MURI began in FY13 and was awarded to a team led by Professor Neal Devaraj at the University of California - San Diego. The goal of this MURI is to understand how biological and biomimetic synthetic cellular elements can be integrated to create novel artificial cells with unprecedented spatial and temporal control of genetic circuits and biological pathways. This research is co-managed by the Life Sciences and Chemical Sciences Divisions.

The field of synthetic biology aims to achieve design-based engineering of biological systems. To achieve this goal, researchers in the field are identifying and characterizing standardized biological parts for use in specific biological organisms. These organisms serve as chassis for engineered biological systems and devices. While single-celled organisms are typically used as synthetic biology chassis, the complexity of even these relatively simple organisms presents significant challenges for achieving robust and predictable engineered systems. A potential solution is the development of minimal cells which contain only those genes and biomolecular machinery necessary for basic life. Concurrent with recent advances toward minimal biological cells, advances have also been made in biomimetic chemical and material systems, including synthetic enzymes, artificial cytoplasm, and composite microparticles with stable internal compartments. These advances provide the scientific opportunity to explore the integration of biological and biomimetic elements to generate an artificial cell that for the first time combines the specificity and complexity of biology with the stability and control of synthetic chemistry.

The objective of this MURI is to integrate artificial bioorthogonal membranes with biological elements to create hybrid artificial cells capable of mimicking the form and function of natural cells but with improved control, stability, and simplicity. If successful, these artificial cells will provide a robust and predictable chassis for engineered biological systems, addressing a current challenge in the field of synthetic biology that may ultimately enable sense-and-respond systems, drug-delivery platforms, and the cost-effective production of high-value molecules that are toxic to living cells (e.g., alternative fuels, antimicrobial agents).

5. Force-activated Synthetic Biology. This MURI began in FY14 and was awarded to a team led by Professor Margaret Gardel at the University of Chicago. The goal of this MURI is to understand the mechanisms by which biochemical activity is regulated with mechanical force and reproduce the mechanisms in virtual and synthetic materials. This research is co-managed with the Materials Science Division.

A critical aspect of synthetic biology systems is the targeted and controlled activation of molecules affecting biological function. Molecules can be activated by a variety of different signals, including chemical, optical and electrical stimuli, and synthetic biological circuits responsive to each of these stimuli have been successfully assembled. In recent years, the ability of mechanical force to serve as a biological signal has emerged as a unique and unexpected facet to biological activation. The rapidly growing field of mechanotransduction is beginning to reveal an extraordinary diversity of mechanisms by which mechanical forces are converted into biological activity. This field has been heavily influenced and driven through ARO-funded research, including a prior MURI.[2-5] Despite these rapid advances, mechanophores have never been incorporated into advanced synthetic material. This research area provides an exceptional opportunity to integrate biological activation by mechanical force into the growing toolbox of synthetic biology, and to establish unprecedented paradigms for the incorporation of highly specific force activation and response into new materials.

The objective of this research is to elucidate the molecular mechanisms by which living cells regulate intracellular biochemical activity with mechanical force, to reproduce and analyze these force-activated phenomena in synthetic and virtual materials, and to design and exploit optimized synthetic pathways with force-activated control. If successful, this research may dramatically influence future advances in engineered biological systems, materials synthesis and fabrication, and force-responsive and adaptive bio-mimetic material systems.

6. Innovation in Prokaryotic Evolution. This MURI began in FY14 and was awarded to a team led by Professor Michael Lynch at Indiana University - Bloomington. The goal of this MURI is to model evolution in nutrient-deprived bacterial cultures, and then characterize changes in the genetic, metabolic, and social networks to create models that reflect the complexities of group evolution.

Classical Darwinian evolution selects for individuals that are better than others of their species in critical areas associated with reproductive fitness. For example, giraffes are selected for longer necks and cheetahs are selected for running speed. Similarly, single-celled organisms growing in rich media are selected for their ability to reproduce more quickly. In contrast, organisms that have run out of food can no longer simply improve at what they are already able to do; they are forced to innovate new methods to exploit previously untapped resources. In times of scarcity, even unicellular organisms rapidly evolve into complex societies with assorted subpopulations formed with unique and specialized skills. It is no longer an effective strategy to grow faster during starvation. In short, evolution during lean times requires the group to evolve as a whole, as each individual competes, cooperates, and depends on other members of the group.

The objective of this research is to develop a model of evolution in isolated independent cultures of organisms that are starving for months or years, and then model change in the genetic, epigenetic, transcriptomic, proteomic, metabolomic, and social networks to create experimentally-validated, mathematically-rigorous, and predictive models that accurately reflect the real complexities of group evolution. In the long term, the results of this research may lead to new applications for safer, economical food and water storage, new mechanisms to control and kill pathogens that will impact wound healing, diabetes, heart disease, dental disease, and gastrointestinal disease.

7. Imaging and Control of Biological Transduction using Nitrogen Vacancy Diamond. This MURI began in FY16 and was awarded to a team led by Professor Ronald Walsworth at Harvard University. The goal of this MURI is to further develop nitrogen vacancy nanodiamonds as non-biological quantum sensors and engineer a biological interface for actuating biological processes. This research is co-managed with the Physics Division.

The nitrogen vacancy center lattice defect in diamond nanoparticles (NV-diamond) can retain activity in biological environments. Current applications of NV-diamond include quantum computing, nanoscale magnetometry, super-resolution imaging and atomic scale magnetic resonance imaging. These state of the art applications involve NV-diamonds implanted in substrates; however recent breakthroughs have allowed isolated nano-diamond particles to be used as biosensing intracellular quantum probes for thermometry and bacterial tracking as well as extracellular quantum probes of ion channel operation. A key reason for NV-diamond sensitivity, including in the emerging biosensing applications, is that the spectral shape and intensity of optical signals from NV-diamond are sensitive to external perturbation by strain, temperature, electric fields and magnetic fields. Biological sensory transduction relies upon highly evolved ion channel-based mechanisms that involve transducing environmental energy into a bioelectrical signal for intercellular communication. The recent

[2] Potisek SL, Davis DA, Sottos NR, White SR, Moore JS. (2007). Mechanophore-linked addition polymers. *J Am Chem Soc*.129:13808-9.

[3] Davis DA, Hamilton A, Yang J, Cremar LD, Van Gough D, Potisek SL, Ong MT, Braun PV, Martínez TJ, White SR, Moore JS, Sottos NR. (2009). Force-induced activation of covalent bonds in mechanoresponsive polymeric materials. *Nature*. 459:68-72.

[4] Lenhardt JM, Ong MT, Choe R, Evenhuis CR, Martinez TJ, Craig SL. (2010). Trapping a diradical transition state by mechanochemical polymer extension. *Science*. 329:1057-60.

[5] Burnworth M, Tang L, Kumpfer JR, Duncan AJ, Beyer FL, Fiore GL, Rowan SJ, Weder C. (2011). Optically healable supramolecular polymers. *Nature*. 472:334-7.

demonstrations of NV-diamond's extreme sensitivity and localization now provide new research opportunities for transitioning NV-diamonds from passive sensors to novel biophysical interfaces whose perturbed energy emission can be used as a signal to control or modify sensory transducer molecular physiology and intra- and inter-cellular signaling.

This multidisciplinary project four closely-coupled aims: (1) to optimize nitrogen vacancy nanodiamond synthesis, (2) to realize stable, biocompatible nanodiamond surface functionalizations, (3) to advance nitrogen vacancy sensitivity to chemical and biological systems and (4) to enable nitrogen vacancy-based manipulation of biological transduction. Systematically studying the integration of nitrogen vacancy nanodiamonds with reconstituted or native ion channels will lead to greater understanding and more importantly, create a new paradigm for exogenous control of biological transduction events and the ability to uncover fundamental mechanisms with unprecedented spatial and temporal resolution. This endeavor may lead to significant scientific breakthroughs in understanding how to develop and control quantum systems capable of interfacing with, and controlling, biological systems. If successful, this research may improve future Army capabilities ranging from advanced artificial intelligence systems, early diagnosis and effective treatment of neurological disorders at the cellular level, novel human-machine interfaces, and antidotes to neurotoxins and pathogens.

8. Sequence-Defined Synthetic Polymers Enabled by Engineered Translation Machinery. This MURI began in FY16 and was awarded to a team led by Professor Michael Jewett at Northwestern University - Evanston. The goal of this MURI is to engineer the translation machinery to accept and polymerize non-biological monomers in a sequence-defined manner using non-traditional chain growth polycondensation chemistries (beyond amide and ester linkages). This research is co-managed by the Chemical Sciences (lead) and Life Sciences Divisions.

Employing only four nucleotides and twenty amino acids, a plethora of biopolymers (e.g., proteins, DNA) with precisely-defined building block sequence gives these materials the ability to fold into higher-ordered structures capable of performing a variety of advanced functions such as information storage, self-replication, and signal transduction. The ability to extend comparable molecular-level sequence control to synthetic polymers, which have a much wider range of monomeric building blocks, has many scientific and technological implications, as it would enable precise control over structure-property relationships. Recent work has demonstrated that altering the sequence of short conjugated phenylene-vinylene oligomers can significantly modulate both electronic and optical properties. While greater complexity in function is anticipated for longer chain sequence-defined polymers, chemical routes to their synthesis have remained elusive. Conversely, biology synthesizes long sequence-defined polymers with extremely high efficiency and accuracy by employing templates to provide sequence information. More specifically, the ribosome, the workhorse of the translation machinery, is very adept at sequence-defined polymer synthesis through the successive condensation of amino acids (monomers), but primarily performs a single type of chemistry—amide bond formation via a chain-growth condensation polymerization. Co-opting the natural translation machinery to accept non-biological monomers is an attractive approach to synthesize non-biological polymers with the sequence control of biology. However, this approach is limited by cell viability constraints; thus, in vitro engineering of the translation machinery may offer unprecedented freedom of design to modify and control ribosome chemistry.

The objective of this research is to engineer and repurpose the translation apparatus (including the ribosome and the associated factors needed for polymerization) to produce new classes of sequence-defined polymers. In the long term, this research may enable a broad range of disruptive technologies having significant impact on DoD capabilities. Sequence control at the atomic level will give the greatest possible control over the emergent, macroscopic behavior of oligomers and polymers, leading to new advanced personal protective gear, sophisticated electronics, fuel cells, advanced solar cells, and nanofabrication, which are all key to the protection and performance of soldiers.

9. Defining Expertise by Discovering the Underlying Neural Mechanisms of Skill Learning. This MURI began in FY16 and was awarded to a team led by Professor Scott Grafton at the University of California – Santa Barbara. The goal of this MURI is to uncover the temporal dynamics of neural substrates and cognitive processes engaged during skill learning and generate a definition of expertise based on the underlying neurocognitive computational advantages generated through learning. This research is co-managed by the Life Sciences (lead) and Mathematical Sciences Divisions.

Neuroscience, social psychology and education are providing insights into neural and cognitive processes involved during skill learning which show structural and functional differences in multiple brain regions when compared between 'experts' and 'novices'. Typically, these comparisons involved a novice time point and an expert time point because of the difficulty measuring intracranial brain activity over the course of skill learning. Novel materials now enable long-term implantation of high density neural recording devices in humans and animal models. Emerging engineering breakthroughs enable spike and local field potential recording from multiple neuroanatomical sites in the brain simultaneously. However, a major analytical barrier prevents easily linking this high density data with data acquired through existing non-invasive electrophysiology techniques and other tools for determining structure-function relationships like magnetic resonance imaging.

The objective of this research is to develop tools and techniques that can both predict and explain from a neurobiological perspective, why there are differences among individuals in their ability to develop expertise. The future force demands expert soldier performance across many tasks. In the long term, this basic research effort will provide a critical foundation for developing training methods based on computational and network neuroscience that are grounded in neurophysiology and neuroanatomy.

10. Dissecting Microbiome-Gut-Brain Circuits for Microbial Modulation of Cognition in Response to Diet and Stress. This MURI began in FY17 and was awarded to a team led by Professor Elaine Hsiao at the University of California - Los Angeles. The objective of this MURI effort is to investigate how the community of microorganisms naturally residing in the human gut (i.e., the gut microbiome) alters cognitive performance in response to nutritional and physical stress.

Recent studies from several laboratories reveal that the responses of the human microbiome, and specifically the gut microbiome, responds to environmental factors (e.g., diet and stress) in a way that modulates host brain activity and behavior.[6-8] The objective of this MURI is to uncover gut microbiome influence on host neurobiology, develop a layered cellular and systems-level model and theory of cognitive and behavioral control by commensal gut microorganisms and extract integrated neural, endocrine, immune and gut microbial interaction principles governing nutrition and physical stress response.

This MURI, if successful, will provide sophisticated predictive tools available to the academic community and DoD upon which more comprehensive biological studies could be performed to more completely understand causative effects throughout this complex networked system. These models have the potential to far exceed current state-of-the-art by offering a currently unavailable analytical framework for future discoveries. The long term potential applications could be the rational design of probiotic regimens to ameliorate symptoms of anxiety-like disorders including PTSD, methods to manipulate the gut microbiome to affect human performance without the need for genetically engineering the human host. Outcomes of this MURI would also direct whole-force recommendations to the Army Surgeon General's Performance Triad and Brain Health Campaigns.

C. Small Business Innovation Research (SBIR) – New Starts

Research within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY17, the Division managed five new-start SBIR contracts, in addition to active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY17 and a list of prior-year topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

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6 Magnusson KR, Hauck L, Jeffrey BM, Elias V, Humphrey A, Nath R, Perrone A, Bermudez LE. (2015). Relationships between diet-related changes in the gut microbiome and cognitive flexibility. *Neuroscience*. 300:128-40.

7 Tillisch K, Labus J, Kilpatrick L, Jiang Z, Stains J, Ebrat B, Guyonnet D, Legrain-Raspaud S, Trotin B, Naliboff B, Mayer EA. (2013). Consumption of fermented milk product with probiotic modulates brain activity. *Gastroenterology*. 144:1394-401.

8 Bravo JA, Forsythe P, Chew MV, Escaravage E, Savignac HM, Dinan TG, Bienenstock J, Cryan JF. (2011). Ingestion of Lactobacillus strain regulates emotional behavior and central GABA receptor expression in a mouse via the vagus nerve. *Proc Natl Acad Sci U S A*. 108:16050-5.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY17, the Division managed four new-start STTR contracts, in addition to active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of STTR topics published in FY17 and a list of prior-year topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Serving Institutions (HBCU/MSI) – New Starts

The HBCU/MSI program encompasses the (i) Partnership in Research Transition (PIRT) Program awards, (ii) DoD Research and Educational Program (REP) awards for HBCU/MSI, and (iii) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY17, the Division managed five new REP awards, in addition to active projects continuing from prior years. In addition, proposals from HBCU/MSIs are often among the projects selected for funding by the Division (refer to the list of HBCU/MSI new starts in *CHAPTER 2, Section IX*.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The following PECASE recipient, previously nominated by this Division, was announced in this fiscal year by the White House. For additional background information regarding this program, refer to Chapter 2: Program Descriptions and Funding Sources.

1. Programing Biomolecular Nanodevices For Targeted Immune Cell Recognition and Payload Delivery. The objective of this PECASE, led by Professor Shawn Douglas at the University of California - San Francisco, is to explore particular DNA structures and determine their affinity for particular cell-surface markers.

This research will design and assemble DNA devices that can identify two types of white blood cells through a suite of markers specific to those cells, and to use these devices to demonstrate delivery of a 'payload' to those cells specifically while ignoring other non-target cells. Achieving the aims of this project would constitute a major paradigm shift for many arenas of human health: in disease treatment for numerous cancers, inflammatory, and autoimmune diseases, as well as in prevention through the ability to selectively enhance immune cells, such as key white blood cells, that are important in fighting off pathogens, parasites, or other invaders to the host system. Military personnel face challenges to their health as a result of foreign travel, close interpersonal contact, stress of combat, and combat-related injury, all of which call for novel approaches to maintaining and optimizing health. The proposed research, if successful, would support the capability for nearly limitless applications focused on changing the behavior of cells through already established biochemical pathways, and for killing unwanted cells through less toxic and more targeted treatments.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY17, the Division managed seven new DURIP projects, totaling $1.3 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. University Affiliated Research Center (UARC): Army Institute for Collaborative Biotechnologies (AICB)

The AICB is managed by ARO on behalf of the Army and is located at the University of California, Santa Barbara (UCSB), in partnership with the Massachusetts Institute of Technology (MIT), the California Institute of Technology (Caltech) and industry. The scientific objective of the AICB is to investigate the fundamental mechanisms underlying the high performance and efficiency of biological systems and to translate these principles to engineered systems for Army needs. Through research and strategic collaborations and alliances with Army laboratories, Research, Development and Engineering Centers (RDECs), and industrial partners, the AICB provides the Army with a single conduit for developing, assessing and adapting new products and biotechnologies for revolutionary advances in the fields of biologically-inspired detection, materials synthesis, energy generation and storage, energy-dispersive materials, information processing, network analysis and neuroscience. A total of $7.7 million was allocated to the AICB in FY17, which was the fourth year of the contract that was amended in FY14 for the next five-year period. Of these FY17 funds, $6.0 million was allocated for 6.1 basic research and $0.5 million was allocated for one 6.2 project.

In FY17, the AICB supported 32 faculty members, 60 graduate students, and 45 postdoctoral fellows across 13 departments at UCSB, Caltech and MIT. The research falls into four Thrusts: (i) Systems and Synthetic Biology, (ii) Bio-inspired Materials, (iii) Biotechnology Tools, and (iv) Cognitive Neuroscience. Detailed descriptions of each core research Thrust and corresponding projects are available at the AICB program website (*http://www.icb.ucsb.edu/research*). A U.S. Army Technical Assessment Board and an Executive Steering Board biennially review the AICB research portfolio, assessing the project goals and accomplishments and set goals for the coming year.

I. DARPA Systems-Based Neurotechnology for Emerging Therapies (SUBNETS) Program

The goal of this program is to create an implanted, closed-loop diagnostic and therapeutic system for treating, and possibly even curing, neuropsychological illness in humans. ARO Life Sciences co-manages SUBNETS projects focused on treatments to restore normal functionality following injury to the brain or the onset of neuropsychological illness. The major approach supported through this program involves clinical trials which will use current FDA-approved implantable intracranial recording devices in neurosurgical patients with psychiatric, epilepsy, movement disorder, and pain conditions in order to identify the corresponding 'signature' network-level brain activity aberrations in these patients. This knowledge will be applied towards a novel treatment strategy based upon a physiologically-defined computational model of neurological circuit function integrated into a closed-loop system. A complementary approach is to develop novel state-of-the-art technology for safe, but high spatiotemporal resolution recording and stimulation to multiple brain regions simultaneously for clinical application. This device platform will far exceed the capabilities of any technology platform ever created and will be available for experimental studies in non-human primates to obtain critical knowledge on mechanisms and will simultaneously inform human clinical studies to validate new recording/stimulation strategies for potential amelioration of human neurological and neuropsychiatric disorders.

J. Defense Forensic Science Center Research and Development Program

The goal of this program, co-managed by the Life Sciences Division and DFSC, is to enhance the capability of forensic science applications in traditional law enforcement/criminal justice purviews and in expeditionary environments. In FY17, eight active projects were co-managed by ARO and DFSC under this program.

One project aims to optimize an RNA-based body fluid multiplex identification system by developing a differential DNA/RNA co-extraction isolation protocol for the separation and analysis of non-sperm and sperm fractions in sexual assault evidence (i.e., prior to DNA profiling and identification of body fluid of origin). The proposed system will enhance forensic capabilities of DFSC and civilian law enforcement by conclusively identifying all forensically relevant biological fluids in a given sample. The proposed system will also be seamlessly compatible with current DNA typing technology by enabling co-extraction of both DNA and RNA from the same forensic sample.

A related effort is taking a protein-based approach to body fluid analysis, using mass spectrometry analysis to detect biomarker proteins specific for forensically-relevant body fluids. Another effort is evaluating ground-, air- and satellite-based sensing technologies for their performance in human grave detection using an experimental study site in east Tennessee, with the main data focus on LIDAR and spectral imaging. The development of remote methods to locate clandestine gravesites will increase gravesite detections per year, reduce recovery cost per individual, and enable the DoD to closely monitor additional gravesites in non-permissive environments, thereby maintaining the grave's chain of custody.

Another effort is developing a Next Generation Sequencing-based autosomal short tandem repeat (STR) allelotyping capability. The proposed platform will enable STR analysis and mitochondrial DNA to be analyzed concurrently, along with other genetic markers that can provide information on the physical characteristics and ancestry of an individual, providing enhanced forensic information to examiners. The development of a set of algorithms and software tools to discover the authenticity and make and model of a digital video's source device by forensically analyzing the video itself is the goal of another project. If successful, this effort would provide a new capability to Army and DoD forensic examiners, as there is currently no scientific method available to make this determination.

Another effort is focused on increasing DoD's ability to identify human remains by creating new kinship and ancestry algorithms that increase the efficiency of identifying old and/or highly degraded remains. The intent of this project is to be able to identify remains of service members when only distantly related individuals are available, as is the case for many remains from WWII, Korea, and Vietnam.

Another project aims to develop a customized laboratory method, interpretation software and reference database for forensic examination of materials to determine geographic origin based on DNA signatures from fungi and plants. This will allow geographic location probabilities to be determined for a given set of fungi or plant spores on a sample. DFSC and DoD personnel (both at crime scenes and in the battlefield) will be able to take advantage of this new system for identifying the geographic origin of an item (e.g., IED, vehicles, and clothing). The final project is developing a spray-on, peel-off, nondestructive coating for trace chemical collection from surfaces and a detailed method for its use. This effort will provide DFSC with an enhanced capability to collect a wide range of trace chemicals from a variety of surfaces, including porous materials which are traditionally challenging to analyze.

K. DARPA Biological Robustness in Complex Settings (BRICS) Program

The goal of this DARPA program is to develop the fundamental understanding and component technologies needed to engineer biosystems that function reliably in changing environments. A long-term goal is to enable the safe transition of synthetic biological systems from well-defined laboratory environments into more complex settings where they can achieve greater biomedical, industrial and strategic potential. Within this program, the Life Sciences Division co-manages one project which seeks to develop new approaches to manipulate unculturable and undomesticated microbes through *in situ* genome engineering. These technologies have the potential to discover new genetically tractable microbes with novel manipulable capabilities for applications in agriculture, bioremediation, bioenergy, biodefense and health. This project further focuses on the development of a generalizable method to limit robustness of the genetic code using overlapping genetic recoding. The results from this genetic study will be useful as a defense against targeted efforts to inactivate a gene or pathway of interest or to remove the engineered safety mechanisms associated with a synthetic function.

L. DARPA Hand Proprioception and Touch Interfaces (HAPTIX) Program

The goal of this program is to create a prosthetic hand system that interfaces permanently with the peripheral nerves in humans. ARO Life Sciences co-manages HAPTIX projects focused on tapping into the motor and sensory signals of an amputee's residual arm, allowing them to control and sense an advanced prosthesis via the same neural signaling pathways used for intact hands and arms. Direct access to peripheral nerves would allow users to move and receive sensation like a natural hand such that it creates a sensory experience so rich and vibrant that users would want to wear their prostheses full time. By restoring sensory functions, HAPTIX also aims to reduce or eliminate phantom limb pain, which affects about 80 percent of amputees. The program plans to adapt one of the prosthetic limb systems developed recently under DARPA's Revolutionizing Prosthetics (RP) program to incorporate interfaces that provide intuitive control and sensory feedback to users. These interfaces build on advanced neural-interface technologies being developed through DARPA's Reliable Neural-Interface Technology (RE-NET) program.

M. DARPA Biological Control Program

The goal of this program is to build new capabilities for the control of biological systems across scales—from nanometers to centimeters, seconds to weeks, and biomolecules to populations of organisms—using embedded controllers made of biological parts to program system-level behavior. The program is co-managed by the Life Sciences Division, which involves participation and leadership in proposal evaluations, selections, monitoring, and site visits. The program is focused on applying and advancing existing control theory to design and implement generalizable biological control strategies analogous to conventional control engineering (e.g., for mechanical and electrical systems). Specifically, the Biological Control program will demonstrate tools to rationally design and implement multiscale, closed-loop control of biological systems, through the development of biological controllers, testbeds to evaluate control of system-level behavior, and theory and models to predict and design effective control strategies. If successful, the resulting advances in fundamental understanding and capabilities will create new opportunities for engineering biology.

N. DARPA Restoring Active Memory (RAM) Replay Program

The goal of this program is to develop new closed-loop, non-invasive systems that leverage the role of neural "replay" in the formation and recall of memory to help individuals better remember specific episodic events and learned skills. ARO Life Sciences co-manages RAM Replay projects focused on non-invasively detecting, modeling, and facilitating real-time correlates of replay in humans, leveraging not only neurophysiology, but also other factors including physiological state and external elements in the surrounding environment. Research challenges include validating assessments and intervention strategies through performance on DoD-relevant tasks, rather than relying on conventional behavioral paradigms commonly used to assess memory in laboratory settings. Using the new knowledge and paradigms for assessing memory formation and recall, the program seeks to improve performance of complex skills by healthy humans.

O. DARPA Rapid Threat Assessment (RTA) Program

The goal of this program is to develop methods and technologies that can, within 30 days of exposure to a human cell, map the complete molecular mechanism through which a threat agent alters cellular processes. The program is co-managed by the Life Sciences Division, which involves participation and leadership in proposal evaluations, selections, monitoring, and site visits. Research challenges include developing tools and methods to detect and identify the cellular components and mechanistic events that take place over a range of times, from the milliseconds immediately following threat agent exposure, to the days over which alterations in gene and protein expression might occur. Understanding the molecular mechanism of a given threat agent would provide researchers the framework with which to develop medical countermeasures and mitigate threats. If RTA is successful, potential adversaries will have to reassess the cost-benefit analysis of using chemical or biological weapons against U.S. forces that have credible medical defenses.

P. DARPA Pathogen Predators Program

The goal of this program is to demonstrate that infections caused by drug-resistant bacterial pathogens and bacterial threat agents might be effectively treated with live predatory bacteria. The program is co-managed by the Life Sciences Division, which involves participation and leadership in proposal evaluations, selections, monitoring, and site visits. The program is focused on answering three fundamental questions about predatory bacteria: (1) Are predatory bacteria toxic to recipient organisms? (2) Against what pathogens are predatory bacteria effective? (3) Can pathogens develop resistance to predation? The potential use of live predatory bacteria as a treatment regimen for bacterial infection would represent a significant departure from conventional antibacterial therapies that rely on small molecule antibiotics.

Q. DARPA INTERfering and Co-Evolving Prevention and Therapy (INTERCEPT) Program

The goal of this program is to determine whether DNA or RNA fragments called therapeutic interfering particles (TIPs) may provide a dynamic approach to providing protection against rapidly evolving viral pathogens. The program is co-managed by the Life Science Division. Conventional vaccine development requires a time-consuming, costly, and inefficient process where the virus' rapid adaptation can result in a vaccine that is ineffective by the time it is released. In contrast, TIPs are viral-derived particles with defective genomes that can only replicate in the presence of the virus, interfering with viral infection through competition for essential viral components. Over the course of this countermeasure-development effort, INTERCEPT performer teams will use novel molecular and genetic design tools, high throughput genomic technologies, and advanced computational methods to address TIP safety, efficacy, long-term co-evolution, and generalizability. If successful, INTERCEPT will deliver new treatments for fast-evolving viruses such as Ebola, SARS, Dengue, Zika, and Chikungunya—providing broad coverage against multiple strains—and make available a platform technology that could be readily adapted to confront even engineered viral threats.

R. DARPA Engineered Living Materials (ELM) Program

The goal of this program is to develop design tools and methods that enable the engineering of structural features into cellular systems that function as living materials, thereby opening up a new design space for construction technology. The program is co-managed by the Life Sciences Division, which involves participation and leadership in proposal evaluations, selections, monitoring, and site visits. The program seeks to develop technologies that enable the engineering of hybrid materials composed of structural scaffolds that support the rapid growth and long-term viability of living cells that endow the final products with biological functions. These materials should exhibit aspects of both the inert grown materials that are being produced today at the factory scale, such as structural integrity, as well as those of living systems, such as self-repair. In addition, the program aims to engineer structural properties directly into the genomes of biological systems, so that living materials can be grown from progenitor cells (e.g., seeds), without the need of non-living scaffolds or external developmental cues. To address this goal, it will be necessary to program developmental pathways that result in multicellular systems with defined patterns and 3D shapes.

S. DARPA Technologies for Host Resilience (THoR)

The goal of this program is to discover biological mechanisms of host tolerance to catalyze the development of novel host-based interventions against emerging pathogens and potential biological threat agents. This program is co-managed by the Life Sciences Division. In the program the investigators seek to develop approaches and methodologies to identify mechanisms of host tolerance along with the characterization of the key biological drivers responsible for that response. The intent is to recapitulate pro-tolerance mechanisms in susceptible hosts by applying a single intervention or a combination of interventions in order to improve readiness and reduce warfighter mortality.

T. DARPA Autonomous Diagnostics to Enable Prevention and Therapeutics

This program seeks to develop new diagnostic devices that decrease the time required to design, manufacture, and rapidly distribute test panels in response to emerging threats. The program also seeks to develop new RNA based platforms for vaccine design and manufacture. It intends to develop new methodologies for rapid engineering of mammalian cells in vivo, including genome-editing tools for cellular manipulation, regulatory elements, and synthetic circuits, and cell sentinel components. Finally, this program also seeks to develop technologies to provide immediate immunity that is rapidly scalable to protect and entire population.

U. DARPA Next Generation Social Science

The goal of this DARPA program is to redefine and recalibrate social science research methods in response to the explosive growth of global digital connectivity, which enables new capabilities for generating large-scale social science experiments under controlled conditions. These capabilities have the potential to engage thousands of participants in small-to-large-scale groups in experimental research and enable the use of new tools, virtual reality in the examination of the dynamics of conflict and cooperation in evolving social groups. This program has the potential to generate path-breaking research designs to improve the capacity to generate causal models of social dynamics, with enhanced reliability, replicability, and reproducibility to determine the factors with the greatest degree of causal influence on emergent social systems.

V. Minerva Research Initiative (MRI) Topic: Studies of Non-State Adversarial Organizations, Ideologies, and Strategies

The focus of this MRI topic is on the relationship among transnational terrorist groups and the fomenting of intergroup conflict. The topic focuses on the interaction of non-state, violent, adversarial groups and existing social, economic, and political systems. Of particular interest is the emphasis on targeted strategies to facilitate the spread of ideology across culturally diverse and global populations through diverse tactics, including the use of news and social media. In addition, this topic investigates both radicalization and de-radicalization of groups through the development of theories of collective action that focus on critical influencers and influence points in social systems. It incorporates both macro computational strategies to generate predictive models of information diffusion and influence, as well as micro models of social biometrics that capture the neural, cognitive, and social pathways that impact social influence. This topic is generating new ways to understand how individuals and groups become susceptible to radical influences, and how different adversarial groups coalesce and fragment over the life of a social movement to enable new ways to detect threats to national security. The BAA for this MRI topic was released each year from FY08-FY17. Project selection and funding began in FY09. There are currently nine projects funded under this topic focus.

W. Minerva Research Initiative (MRI) Topic: Sociality, Security, & Interconnectivity

The objective of this MRI topic is to examine the relationship among culture, social conflict, and social organization, with an emphasis on shifts in existing global order as influenced by population inequalities and demographic shifts , with particular attention to global powers including (but not limited to) the United States, China, and Russia and the relationships among these powers, how they intervene in global politics, and how increasing global interconnectivity influences the sociopolitical dynamics across global networks. If successful, this research will facilitate the identification of emergent power dynamics that shape global sociopolitical dynamics, identifying the content and structure of relationships, capacity to assess emergent threats across inter-state networks of actors, and generate new insights on the strategies of influence in global politics. The BAA for this MRI topic was released in FY16 and funding began in FY17. There are currently six projects funded under this topic focus.

X. Minerva Research Initiative (MRI) Topic: Societal Resilience

This MRI topic investigates the social, cultural, and political dynamics that shape a society's capacity to overcome adversity as posed by natural disasters, public health threats, and human-constructed crises, including war, socioeconomic inequality, sociopolitical violence. These threats often set the stage for major upheavals and introduction of adversarial forces. The topic examines migratory patterns and responses to displacement of major populations, impact of migration on in- and out-migration regions on cultural conflict in receiving states and states from which populations are fleeing. In addition, this topic focuses on the how social institutions (e.g.,education, economic, governance, kin, religion) adapt to shocks resulting from crises, mechanisms to improve capacity to respond and re-stabilize social systems. It includes development of new databases on the predictors of state fragility and communication strategies that enable recovery. Additionally, this topic area will engender new approaches to multilevel and multiplex modeling of complex systems to generate new insights on the factors that facilitate rapid re-stabilization. Finally, this topic emphasis will promote development of new capabilities to both predict at-risk areas and sense impending threats to resilience enabling improved potential for early intervention in populations at risk of adversarial influences that pose national security risks. The BAA for this topic was released in FY16 and funding began in FY17. There are currently six projects funded under this topic focus.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Life Sciences Division.

A. Attenuation of Polyglutamine-induced Toxicity by Enhancement of Mitochondrial Oxidative Phosphorylation

Professor Antoni Barrientos, University of Miami, Single Investigator Award

The objective of this research is to identify and characterize the basic molecular and metabolic alternations that occur during aging of post-mitotic cells such as neurons under proteotoxic stress. One hallmark of an aging organism is the accumulation of defects in mitochondria. As mitochondria accumulate mutations their energetic capability becomes diminished and they leak ever increasing amount of free radicals, which in turn cause more mitochondrial damage as well as damage to nuclear DNA and intracellular proteins. Defects in mitochondrial biogenesis and function are also common in many neurodegenerative disorders including Huntington's disease.

The investigators demonstrated that Hap4, the catalytic subunit of the transcriptional complex that regulates mitochondrial gene expression, alleviates the growth arrest induced by expanded polyglutamine tract peptides in rapidly dividing cells. They also demonstrated that the protective effects of Hap4 overexpression require mitochondrial respiration and oxidative phosphorylation. Furthermore they demonstrated that enhancement of mitochondrial biogenesis protects against the neurodegeneration and behavioral deficits associated with Huntington's disease. These results suggest that therapeutic interventions that enhance mitochondrial respiration and oxidative phosphorylation could reduce the toxicity of expanded polyglutamine tracts and delay the onset of Huntington's disease. This also suggests potential therapeutic approaches to protect warfighters against the effects of damaged mitochondria as they age. This effort is part of a larger ARL-wide thrust to improve warfighter performance.

B. Design of Protein Biomaterials Through Tailored Shape and Packing Strategies of Patchy Particles

Professor Andy Ellington, University of Texas – Austin, and Professor Sharon Glotzer, University of Michigan, Single Investigator Award

Using folded protein molecules as nanoparticle building blocks is a promising strategy to explore the tremendous design space of functionalized biomaterials. Surprisingly little general knowledge is available on the forces that drive the formation of ordered protein assemblies, and much of the available knowledge is of empirical nature. Broadly, the reason for this lack of fundamental understanding is due both to the plethora of different native structures into which proteins fold, and the richness in their chemical identities. Physical interactions involved in structure formation can arise from hydrophobic interactions, charged surface patches or steric exclusion, such as the lock-key principle. While there are isolated examples of complex protein-based structures that assembled as designed, accompanying theoretical calculations that would aid in the prediction and design of higher-order protein-based structures has been lacking. In contrast, for colloidal systems, robust theory has been developed that describes the assembly of hard particles with defined shape and patchy interaction surfaces.

In a joint effort, Professors Andy Ellington and Sharon Glotzer aim to apply the understanding of the assembly of model colloids to the design of a protein-based structure with defined functionality. Using fluorescent proteins as a model system, the research team aims to predict specific surface substitutions that will lead to thermodynamically stable packings that can be engineered and validated using biophysical methods. Specifically, the team proposes a new 'patchy shape' modeling approach, which combines features of more atomistic approaches with the idea of a coarse-grained protein representation. This modeling approach will aim to represent proteins by their three-dimensional native shape including attractive surface patches. The coarse-grained model will then be refined using molecular docking simulations. Ordered aggregates of green fluorescent protein (GFP) and variants, such as cyan or yellow fluorescent protein, with defined morphology and molecular orientation will be designed using the patchy shape modeling approach. The proposed designs will then be evaluated experimentally through surface residue modifications that result in supercharged GFP variants.

Ordered aggregates successfully assembled in the lab will be characterized using light scattering to test for aggregation, differential scanning fluorimetry to assess thermal stability, and fluorescence resonance energy transfer and microscopy to validate the structure. The mechanical properties of stable aggregates will be analyzed using rheology.

In FY17, the research team successfully designed supercharged GFP variants that assemble into a defined higher-order structure. Two GFP variants were mixed to promote assembly of the structure, one with a net positive charge and one with a net negative charge. The team then identified conditions favoring the formation of ~11 nm diameter "protomers" that further assembled into micron-scale particles (see FIGURE 2). Overall, this approach of supercharging protein surfaces may ultimately prove to be a robust means of assembling biomolecules into materials with internal ordered structure.

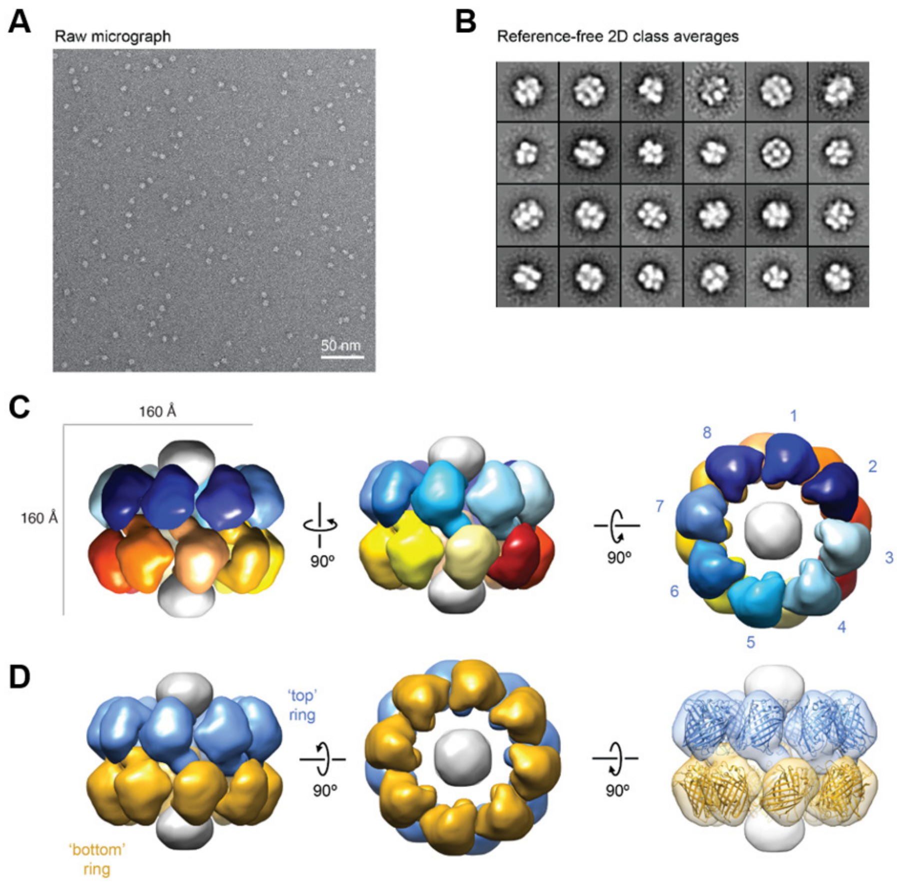

FIGURE 2

Molecular architecture of the GFP protomer. (**A**) Raw cryo-electron micrographs of assembled particles of positively and negatively supercharged GFP variants. (**B**) Reference-free 2D class averages of the GFP protomers shown in (A). (**C**) Three-dimensional architecture of negatively stained GFP protomer at ~18-Å resolution with 8 subunits forming an octameric ring. (**D**) Each protomer consists of a top and bottom ring that are offset by ~0.5 subunits in the axial direction. The x-ray crystal structure of GFP is easily accommodated within the map of each of these subunits.

The scientific understanding being illuminated by this effort will lay the scientific foundation toward development of engineered biomaterials with interactions and properties that predictably span the atomic to macro-scale. This understanding has potential to significantly accelerate the development of several Army-relevant materials.

C. Defining How Culture Conditions Influence Mutation

Professor T. Ferenci, University of Sydney, International Technology Center (ITC) Single Investigator Award

The inevitability of mutational changes is a threat to the stability of future synthetic biology constructs. Models so far have assumed a random generation of mutational events over time. Professor T. Ferenci and collaborators investigated the role that different culture conditions, in the absence of selective pressure, can have in determining mutational types and rates. Using *E. coli* chemostat cultures, five different environmental stresses (carbon, phosphate, nitrogen, oxygen, or iron limitation) were investigated, in addition to the unlimited-nutrient control condition. They found each limitation to be associated with a distinct mutational profile, including distinct effects on the repair proteins that work to limit or prevent mutation. The team reported that the unexpected diversity of input-output effects explains some important phenomena in the mutational biases of evolving genomes, and that environments influence genetic variation as well as selection (see FIGURE 3).[9]

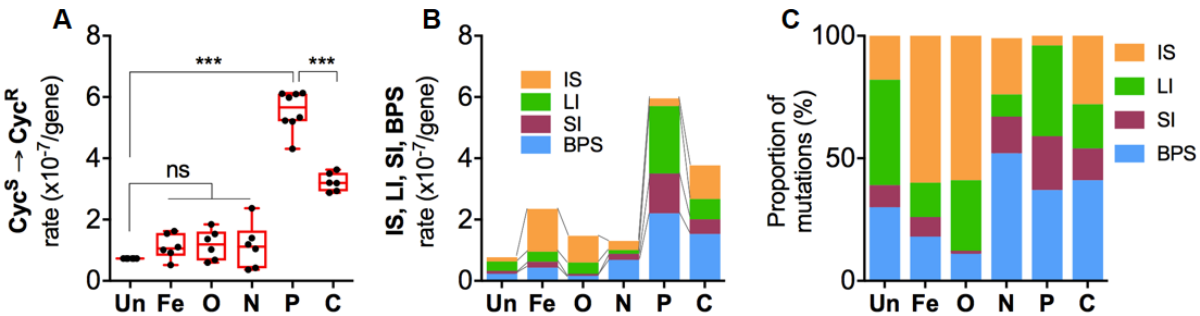

FIGURE 3

Mutation rate plasticity and fitness in six culture environments. (**A**) Mutation rates were calculated from the frequency of cycloserine resistance (CycR) mutants appearing in cycloserine-sensitive (CycS) cultures of E. coli for 6 replicate populations in each of 6 different nutritional states: Un (nutrient-unlimited), iron (Fe) limited, oxygen (O) limited, nitrogen (N) limited, phosphorous (P) limited, and carbon (C) limited. (**B**) Different color bars represent the mean mutation rates of the 4 major classes of mutations (base-pair substitutions [BPS], single base pair indels [SI], deletion and insertion indels > 1bp [LI], and insertion sequence [IS] transpositions). (**C**) The colored bars represent relative contribution of BPS, IS, SI, and LI classes to the total mutation rate within each of 6 environments, shown as a proportion of total mutations.[8]

D. Role of Protein Aggregation and Persistence in Promoting Desiccation Survival in Bacteria

Professor Bryan Davies, University of Texas - Austin, Single Investigator Award

Desiccation is a stressful condition for survival of non-spore forming bacteria due to cellular dehydration and the ensuing molecular damage and loss of energy stores. The loss of activity from damage repair enzymes can increase the level of oxidative stress and inhibit the ability of the cell to repair itself. It is thought that bacteria can survive desiccation by lowering their metabolic state thereby conserving energy and reducing cellular damage. Toward an understanding of the factors that promote desiccation survival. Through genetic screening and transcriptomics it was found that desiccation appears to activate toxins of the same putative toxin-antitoxin modules that are active during the state of bacterial persistence within antibiotic tolerant cells. Professor Davies' research is using the model Gram-negative bacteria *Acinetobacter baumannii* to comprehensively characterize the function and regulation of putative toxin systems governing this organism's desiccation survival and their global effect on translation (see FIGURE 4). As persistence is marked by a severe reduction in translational capacity and hence a lower metabolic state, it is thought that the same mechanisms that allow for survival in antibiotic-tolerant cells may also work toward maintaining viability during desiccation.

The transcriptomic study further showed that desiccation markedly changes the expression level of genes related to protein translation or stability. As proteome stress often causes proteins to misfold and aggregate, it was hypothesized that dehydration will cause proteins to misfold due to a lack of water thereby increasing aggregation level. To test this hypothesis, Professor Davies assayed for protein aggregation levels in desiccated samples and compared to samples under normal growth conditions. Working with a variety of different growth

[9] Maharjan RP, Ferenci T. (2017). A shifting mutational landscape in 6 nutritional states: Stress-induced mutagenesis as a series of distinct stress input–mutation output relationships. *PLoS Biol* 15: e2001477.

conditions that are marked by noticeable differences in desiccation survival, he first demonstrated that desiccation survival correlated with the level of protein aggregation. To further verify this correlation, Davies treated *A. baumannii* cells grown in log phase with a 30 min pulse of streptomycin, a ribosome-targeting antibiotic that induces protein aggregation by increasing protein mistranslation; as expected, the levels of both the aggregates and percent survival under desiccation increased after streptomycin treatment. Finally, Davies demonstrated that these protein aggregates can refold reversibly; lacZ protein bound in these aggregates was functionally revived when incubated with lysates of wild-type *A. baumannii*.

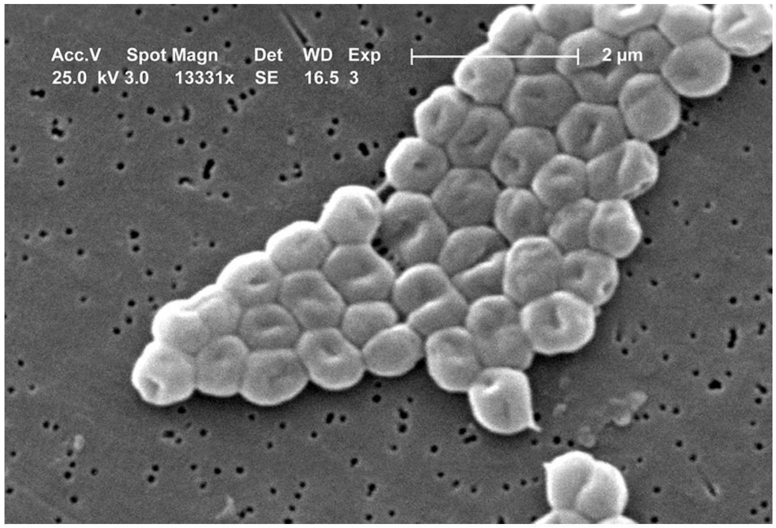

FIGURE 4

Gram-negative non-spore forming species *Acinetobacter baumannii* has been characterized as a bacterium that survives under conditions of desiccation.

These results indicate that aggregates may represent a means for *A. baumannii* to store proteins, protect them from desiccation damage and revive them in functional form once better growth conditions have returned. Further studies will pursue the link between toxin activity and the formation of these aggregates. A clearer understanding of the molecular mechanisms that allow bacteria to survive the extreme stress of desiccation will provide the Army with effective design strategies for the use of field-based microorganisms as reporters, sensors and platforms for biosynthesis in challenging environments.

E. Sensorimotor Function in Elite Athletes

Professor Lawrence Appelbaum, Duke University, Single Investigator Award

Highly experienced soldiers and athletes are experts at processing visual information and therefore developing an understanding of how their visual skills differ from others can inform models of learning while also uncovering the upper bounds of human ability. The goal of this research is to perform secondary analysis of data collected through a large-scale sensory performance program that includes measures of vision, cognition, and visual-motor control in hundreds of soldiers and thousands of athletes at all levels of achievement. Exploring variability in sensorimotor abilities over this large and unique population will help to uncover how visual skills relate to athletic and military expertise, real-world achievement, and resilience to traumatic brain injury.

Professor Appelbaum's research focuses on analysis of past and future data collected with the Nike Sensory Station, a reliable and cross-validated computerized assessment device that measures nine sensorimotor skills and has already collected data from thousands of soldiers and athletes at all levels of achievement. In FY17 Professor Appelbaum completed analyses on the available psychometric and demographic data, sports statistical data, and baseline concussion data assembled and organized from the large multi-center database of soldiers and athletes. He also led the opening of the Sports Vision Center to serve as a new data collection site for college and professional athletics at Duke.

Using prospective analyses, he tested the hypothesis that sensorimotor skills are predictive of game statistics for specific on-field athletic positions, thereby advancing knowledge about which aspects of sensorimotor skills are valued for real-world success. Professor Appelbaum's analyses recently revealed better performance for hitters relative to pitchers at the professional level in visual clarity and depth perception, but these differences did not exist at the high school or college levels, indicating that professional-level hitters have better visual acuity and depth perception than professional-level pitchers (see FIGURE 5). This work affirmed the notion that highly experienced athletes, based on their positions, have differing perceptual skills and identified specific psychomotor and sensorimotor behavioral skills that predict on-field performance.

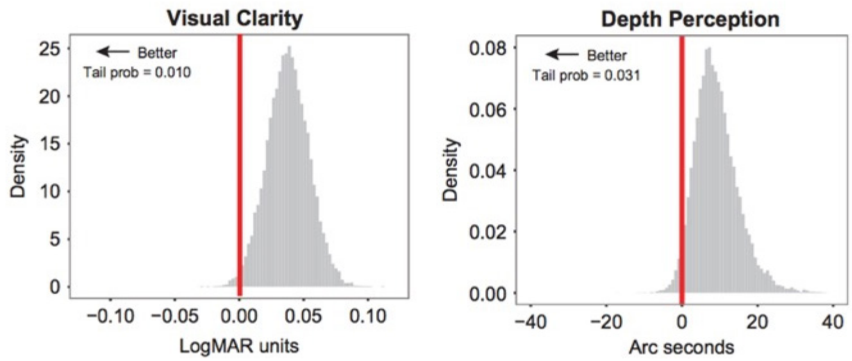

FIGURE 5

Hitters show better performance than pitchers in visual perception tasks. Posterior position effect distributions for the visual clarity and depth perception tasks, comprised of 21,000 samples comparing pitcher-minus-hitter differences collected on the Nike Sensory Station. Red vertical lines indicate no difference (zero) between pitchers and hitters. Arrows indicating the directions of "better" performance for hitters and the tail probabilities are shown for each task. These results demonstrate better performance for hitters relative to pitchers on these tasks, while no differences were present in 7 other visual tasks.

In FY18 Professor Appelbaum's team will continue data collection from the Nike Sensory Station database and identify additional statistical relationships between sensorimotor skill and real-world performance within and between specific groups of military and athlete cohorts to develop a detailed understanding of how different sensory demands relate to better or worse sensorimotor skills. The present research offers a unique and cost-effective opportunity to explore unknown relationships between specific cognitive and sensorimotor skills and performance in a large sample of high-achieving soldiers and athletes while they demonstrate real-world performance, opening the possibility for new cognitive-physical performance standards for Soldier assessment.

F. Vocal Accommodation within Nonverbal Frequencies as a Marker of Status, Dominance, and Prestige

Joseph Dippong, University of North Carolina - Charlotte, Young Investigator Program (YIP) Award

Social influence is a subtle process that arises from status processes that organize social groups. It determines collective action at both local levels (e.g., functioning of teams) and global levels (e.g., policies of nations). Moreover, it often arises from demographic attributes of group members such as age, race, gender, which are frequently irrelevant to tasks confronting groups compared to factors such as experience, expertise, and developed skills. Demographic attributes are referred to as diffuse status characteristics, while particular skill- and experience-related attributes are referred to as specific status characteristics.

Research by Professor Joseph Dippong and others has consistently shown that social influence often arises strictly from diffuse characteristics, despite their irrelevance to a problem a collective is attempting to solve. Determining when social influence is being exercised is critical to predicting whose position will dominate in a group, what course of action a group will take, and the extent to which a collective will confront resistance. Yet, tracking social influence as it emerges within and across groups has remained a challenge, partly due to the reliance on subjective self-reports and *post hoc* accounts of influence processes. Professor Dippong has developed new methods to capture influence as it evolves based on non-intrusive measures of dominance of lower frequencies of the vocal spectrum (see Figure 6). While all actors modulate the frequency of their vocal patterns across exchanges with one another in both small groups and large collectives, Professor. Dippong's research has demonstrated that in collectives, the actor who dominates the low voice spectrum corresponds with the most influential actor and actors whose demographic attributes (even when irrelevant) place them in higher status positions. Moreover, prior research that shows that social information is carried in this component of the vocal spectrum, which is difficult to consciously control. In addition, the actual content of the communication carried in this range of the vocal spectrum is not comprehensible (it is essentially commensurate with hearing the murmuring of a conversation through a well-insulated wall), suggesting important pathways of neural processing that this spectrum involves. He has further demonstrated that lower status actors will cede control of this region of the vocal spectrum to higher status actors during the course of interaciton, corresponding to increasing influence by the higher status actors. The research provides a new approach to understanding the biophysiological foundations of social interaction and influence, enabling new non-intrusive methods for detecting the evolution of social influence.

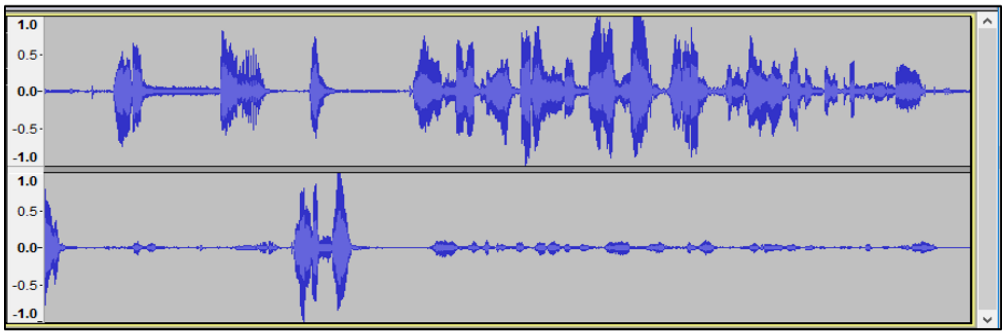

FIGURE 6

Vocal Accommodation. This figure shows exemplary data from the low voice spectrum of two individuals engaged in conversation during a decision-making task. The top panel depicts the higher status individual's low-vocal spectrum patterns, whereas the lower panel shows the lower status individual's low vocal spectrum patterns. Comparison of the two patterns demonstrates the consistent finding that higher status actors dominate the low voice spectrum, compared to higher status actors and that as interaction progresses, higher status actors gain increasing dominance in this part of the voice spectrum.

G. Biophysiological and Social Predictors of Political Violence

Professor William Reed, University of Maryland, Single Investigator Award

Understanding factors that contribute to individual propensities for violence remains an ongoing concern of the security community. There has been considerable work on institutional and economic factors that may drive individuals toward violent actions, but why inequalities and repression drive some toward violence but not others has been a challenging problem for scientists to explain. Professor William Reed's research demonstrates the importance of biophysiological factors. Specifically, his research aims to explore genetic variation in two genes, MAO-A and 5-HTT, which have been linked to aggression in adulthood that is correlated with early childhood trauma. Professor Reed developed and tested a sophisticated diathesis-stress showing how a specific genetic vulnerability, in this case inefficiency in serotonin transportation resulting from low MAO-A/short 5-HTT alleles, when combined with an environmental stressor, such as repression, increases rates of particular behaviors, in this case violent aggression (see FIGURE 7). This approach is addressing past shortcomings in research on genetic determinants of social behavior that have not been able to account for environmental conditions that are critical to genetic expression. Moreover, it represents the first systematic attempt to link gene x environment interactions to political violence.

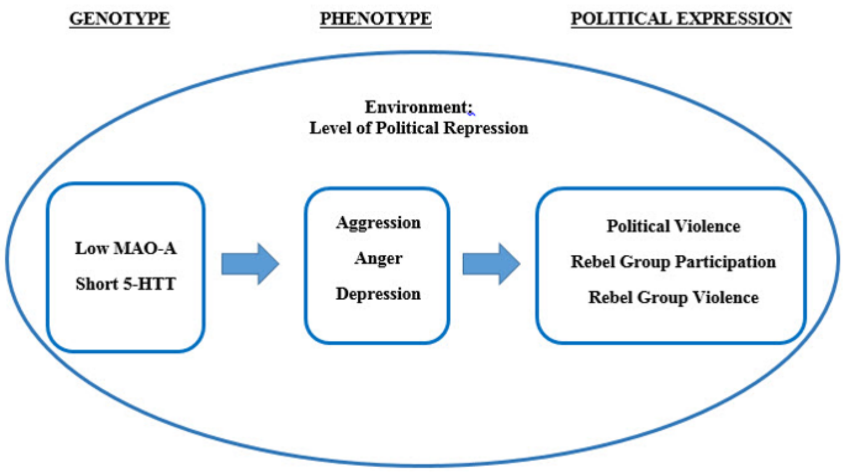

FIGURE 7

Causal model depicting path from genetic variation to engagement in violence. Research in political sciences has traditionally focused on the right box in the diagram, with challenges in explaining substantial individual variation in these behaviors. Integrating political science approaches with behavioral genetics addresses this challenge.

Professor Reed has collected and analyzed genetic samples from a sample of combatants and non-combatants within particular social groups, along with survey data on past and current experiences with political repression, inequality, and forms of political participation, including involvement in violent responses. A matched sample of groups from other social collectives was included to overcome a common issue in candidate gene association research in which focus on particular populations creates confounds in the analytic results. Through a series of experiments, Professor Reed's laboratory found that individuals with the low MAO-A allele had heightened aggressive tendencies when exposed to injustice and were more likely to report engagement in political violence, compared to those with the low MAO-A allele (see FIGURE 8). Furthermore, the research demonstrates that those with the low MAO-A allele exhibit greater degrees of impulsive decision-making compared those with the high MAOA allele. The research has demonstrated critical new advances on gene x environment interactions, highlighting the importance of social conditions in triggering pathways to violence through impulsiveness and aggression, offering new potential to quell violence by predicting it before it emerges and developing interventions to address the social factors that spur violence.

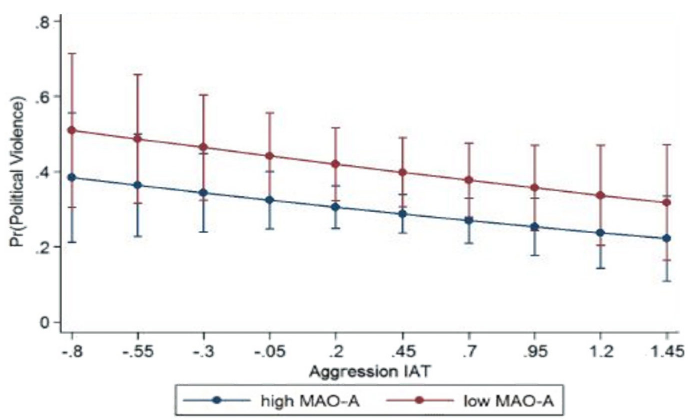

FIGURE 8

Effects of aggression tendencies on political violence. Research in political sciences has traditionally focused on the right box in the diagram, with challenges in explaining substantial individual variation in these behaviors. Integrating political science approaches with behavioral genetics addresses this challenge.

H. Engineering Live Cell Surfaces with Functional Polymers

Professor Craig Hawker, University of California - Santa Barbara, AICB (UARC)

The capability to graft synthetic polymers onto the surfaces of live cells offers the potential to manipulate and control their phenotype and underlying cellular processes. Compared with small molecule cell surface modifications, grafting synthetic polymers provides a number of advantages associated with the increase in functional groups available for secondary interactions, derivatization, and changes in physical properties.

In FY17, Professor Hawker and colleagues reported the first cytocompatible, visible light-mediated strategy for generating structurally defined synthetic polymers on live yeast and mammalian cell surfaces.[10] Polymerization initiating chain-transfer agent groups were introduced on the cell surface using either a covalent (yeast) or a non-covalent insertion strategy (mammalian). When compared to traditional approaches, the increased efficiency of polymer grafting in these systems enabled the cellular phenotype to be manipulated by deliberately inducing aggregation and assembly in the presence of tannic acid (see FIGURE 9). Given that these methods could be readily expanded to graft a range of functional polymers onto cell surfaces, they may enable an array of applications including rewiring of signaling pathways and controlling cell–cell interactions.

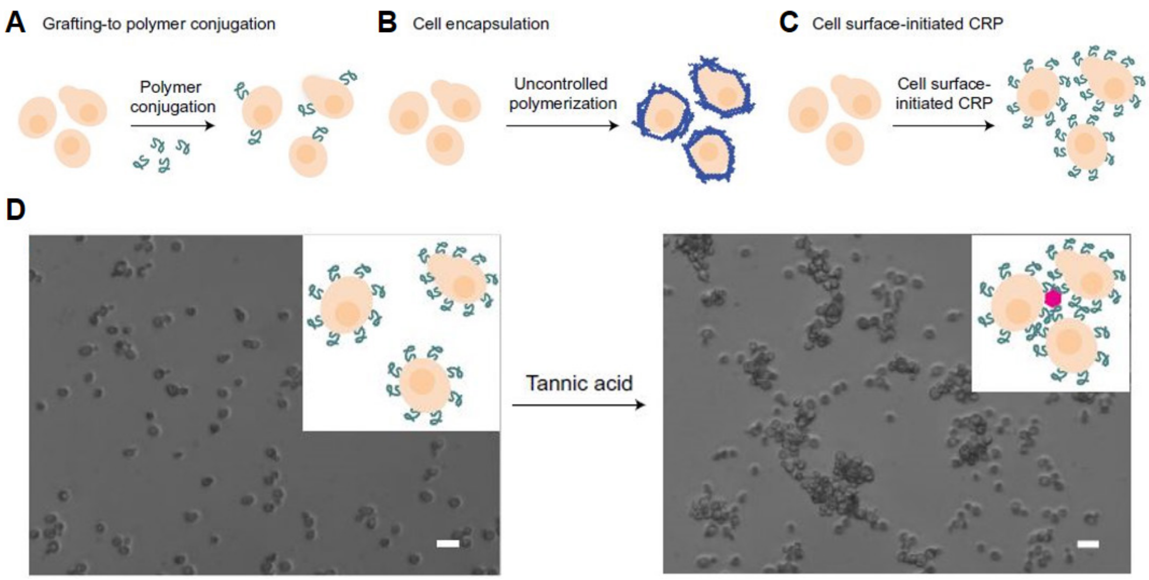

FIGURE 9

Strategies for engineering cell surfaces using synthetic polymers and manipulation of cellular phenotype. Grafting-to methods (**A**) tend to suffer from low grafting densities, whereas, existing grafting-from methods (**B**) based on cell encapsulation do not enable control over the extent or structure of the grafted polymers. The controlled radical polymerization (CRP) method (**C**) offers a biocompatible technique for controlled addition of high densities of functional polymers to cell surfaces. (**D**) Micrographs and illustrations of changes in cell morphology: tannic acid (TA), which can bind to PEG through hydrogen bonding interactions, was introduced to mediate aggregation of polymer-modified yeast cells. Bright-field microscope images show before and after TA treatment. Scale bars are 5 μm.

[10] Niu J, Lunn DJ, Pusuluri A, Yoo JI, O'Malley MA, Mitragotri S, Soh HT, Hawker CJ. (2017). Engineering live cell surfaces with functional polymers via cytocompatible controlled radical polymerization. *Nat Chem.* 9:537-545.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Multi-scale Dynamics of Cortical Adaptation for Human Auditory Detection

Investigator: Professor Dana Boatman, Johns Hopkins University, Single Investigator Award
Recipient: ARL-HRED

Results from single investigator-funded researcher Dana Boatman at Johns Hopkins University have transitioned to ARL-HRED to facilitate diagnosis and treatment of blast-induced mild traumatic brain injury in Service members. The originating research objective is to develop a multi-compartmental model to simulate local cortical activity in the auditory cortex, including firing patterns, in order to model data from human electrocorticography recordings during active listening in awake human subjects (see FIGURE 10).

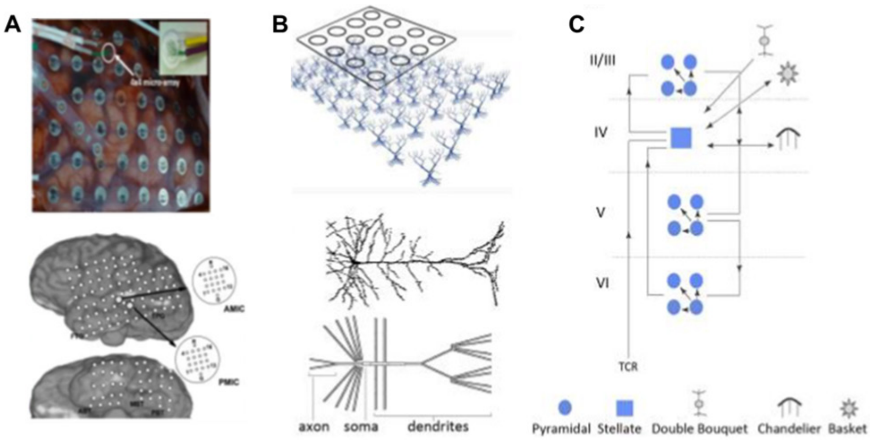

FIGURE 10

Human electrocorticography and cortical modeling. (A) Intra-operative photo of electrocorticography grid array placement. Bottom, left hemisphere lateral and mesial 3D MRI reconstruction showing implanted arrays and coverage of superior temporal gyrus. (B) Schematic of Layer II/III neuronal network in modeled minicolumn with modeled micro-elements above to represent 4x4 micro-electrode recording array on cortical surface. Note: inter-cell and inter-electrode distances are rescaled for visualization; actual scale factor ratio is approximately 50:1. Bottom, in vivo pyramidal cell (top) and modeled pyramidal cell (bottom). (C) Diagram of cellular architecture and connectivity in modeled minicolumn. Omitted for visibility are: Layer IV pyramidal cells, Layer I containing pyramidal apical dendrites from Layers II/III; inhibitory connections to other layers, and thalamic reticular nucleus input.

In FY17, Professor Boatman and colleagues further developed a mathematical model of brain cortical activity that has led to new insights about brain dynamics. This multicompartment model transitioned to ARL Human Sciences Campaign Scientists to support research intended to elucidate the multiscale changes in neural circuits to identify the mechanisms of cognitive decline due to exposure of Service Members to primary explosive blast. Working in concert with JHU researchers, ARL-HRED scientists have for the first time established how the large-scale deficiencies in sensory processing that are found in mild brain injury cases can result from neuronal damage at the cellular level. Through simulation studies, the teams were able to predict how damage to a single neuron can spread to larger communication within neural networks. This new understanding is particularly needed in cases where morphological abnormalities are not detectable through commonly-used diagnostic techniques, such as Magnetic Resonance Imaging.

B. Artificial Cells for Novel Synthetic Biology Chassis
Investigator: Professor Jeff Hasty, University of California - San Diego (UCSB), MURI Award
Recipients: ARL-SEDD, ECBC, AFRL, NRL

Mastering the capabilities of living systems is a scientific grand challenge that could catalyze the discovery, design, and synthesis of new materials. Biomimetic research has long aimed to create artificial cells consisting of minimal biochemical elements yet capable of performing functions with the extraordinary ability of naturally occurring cellular systems. An attractive route is to develop hybrid cells consisting of artificial supramolecular structures fully integrated with biological elements. Such artificial cells would be able to incorporate the toolbox of synthetic biology, such as genetic circuits and exquisitely evolved biochemical pathways, while possessing the stability, organization, and predictability of purely synthetic systems. A MURI team led by Professor Neal Devaraj is exploring the assembly of an artificial cell by integrating artificial chemical membranes with encapsulated dynamic gene networks and engineered molecular transport mechanisms to create hybrid "cells" capable of mimicking the function of natural cells but with improved control, stability, and simplicity.

As part of this MURI program, Professors Hasty and Tsimring, co-PIs at UCSB, and their research team developed a method for extracting cellular material from bacteria that, when combined with the latest tools in synthetic biology, may provide for more rapid and accurate field sensors for pathogens, toxins, or chemical agents. The cellular extract of modified bacterial cells is a powerful tool in molecular and synthetic biology; however, the preparation methods for obtaining these extracts are complex, labor intensive, and costly, and yield short-lived and fragile material. The research team developed a method for preparing active cellular extract three times faster and at less cost than previous methods (see FIGURE 11).[11] The team then demonstrated the use of these extracts in detecting a mercury-based toxin, showing that this method is suitable for on-demand use in subsequent experiments and in the development of future applications.

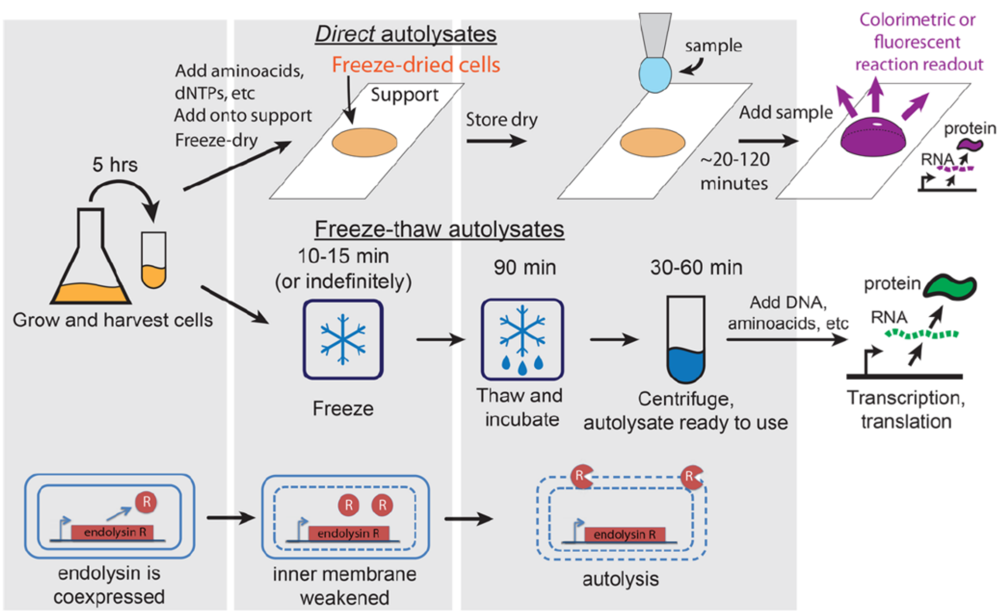

FIGURE 11

Overview of autolysate preparation. The autolysis plasmid constitutively produces low levels of phage lambda endolysin (gene R). The presence of endolysin has no significant effect on cell growth as long as the inner cell membrane is intact. These cells are then used to prepare cell autolysates either by freeze-drying and rehydration or by freeze−thawing (see the top and middle panels respectively). Gene circuit DNA and/or an analyte of interest can be added during rehydration. The reaction readout can be performed using fluorescent, colorimetric, or other output. Upon thawing the cells lyse, and the cell extract is ready to use after 90 min "run-off" incubation at 37 °C and centrifugation to remove insoluble material. Transcription and translation are initiated upon addition of the desired plasmid DNA and standard reaction constituents.

[11] Didovyk A, Tonooka T, Tsimring L, Hasty J. (2017). Rapid and Scalable Preparation of Bacterial Lysates for Cell-Free Gene Expression. *ACS Synth. Biol.* 6:2198-2208.

This method transitioned to the Synthetic Biology for Military Environments (SBME) Applied Research for the Advancement of S&T Priorities (ARAP) program for evaluation by S&Es in ARL-SEDD, ECBC, AFRL and NRL for integration with cell-free synthetic biology research efforts under this program. The long term Army impact of this research is expected to be the cost-effective and rapid production and screening of high-value molecules such as alternative fuels or pharmaceuticals, and the development of portable platforms to detect pathogens or chemical warfare agents at increased speed and decreased cost relative to existing methods.

C. Rebel Contraband Database Utilized by Analysts to Assess Security Risks
Investigator: Professor James Igoe Walsh, University of North Carolina, Charlotte, Minerva Award
Recipient: Defense Intelligence Agency

Violence enacted by non-state adversarial groups, including violent terrorist organizations requires considerable resourcing to fund activities. The sources of funds, however, have been difficult to identify,, as are the consequences for the communities from which the funds are obtained. Anecdotally, it has been believed that some communities and social groups are complacent when resources are transferred to violent groups, and at other times they are resistant. The reasons for these different orientations toward rebel groups have been theorized but not tested because of lack of valid data. Furthermore, validated data and models of how these transfers occur has been elusive.

ARO-funded research conducted over four years by Dr. James Walsh has generated new methods using triangulated information from different publicly available sources to generate a validated dataset documenting how rebel groups seize and receive natural resources (e.g., oil, minerals, agricultural goods) that confer to other resources (e.g., money, materials) to support violent efforts. The methodology includes using gesparsing and geoevent coding techniques that are language agnostic to rapidly extract and analyze data from a variety of unstructured documents (e.g., news reports, social media). Importantly, this analyses of the data and models developed by Dr. Walsh also shows that in some instances, the resources are willingly transferred because the adversarial groups are addressing critical needs of the population that controls them that are unmet by state actors and groups. The database (which captures violence and resource transfers starting in 1990) has been shared with the Defense Intelligence Agency, which is using it to better understand the strategies rebel groups use to obtain resources to support activities, identify at-risk regions for such activities, and develop mitigation strategies.

D. Research on Western Jihadists Networks Informing Analysis of Ties between Terrorist Groups
Investigator: Professor Jyette Klausen, Brandeis University, Single Investigator Award
Recipient: National Security Agency

Violent social movements, such as radical violent Jihadist organizations, have commonly been considered to be relatively independent groups, lacking formalized ties across them. Yet, there are striking similarities across some in the tactics they use in large-scale attacks. In the past, researchers believed this was due to diffusion of information through informal and public channels (such as the media). Determining whether purposeful or formal linkages across violent extremist organizations exist is challenging because most of these organizations operate on what is referred to as “dark networks” – essentially underground groups with little to no public identities or exposure. Consequently, tracking their interactions is extremely challenging.

Professor Klausen has developed novel approaches to develop maps of dark networks. In particular, the research entails examining near-neighbors’ ties and actions in a network obtained by combining data sources including social media, news reports, arrest records, and other public data. The approach entails a multi-urn methodology to extract the information from these sources to build the datasets. The critical advance Klausen has made is in using not the top-level information (e.g., who is communicating with or tracking whom on social media), but rather the information that captures deviance in this information (e.g., suspended social media accounts, arrest records, elimination individual records). These data can then be traced to emergence of alternative records and identities, revealing otherwise undocumented networks. The project has tracked over 6,000 actors, 797 terrorist plots, and 23,000 links between persons and persons and organizations in dark networks. The data generated by this project transitioned to the National Security Agency, Laboratory for Analytic Sciences to enable analysts to continue to analyze the data, identifying potential new networks of violent extremists and violent extremist organizations. The data and reports of the research have also been shared with the U.S Department of Justice.

E. DNA Barcoding for Forensic Palynology

Investigators: Professor Berry Brosi, Emory University, Single Investigator Award
Recipient: Defense Forensic Science Center

The use of pollen to identify the geographic origin of items of interest has been limited by the need for an expert palynologist to interpret the results, the weeks required to individually identify grains of pollen under a microscope, and the relatively poor taxonomic resolution possible from phenotypic identification. While DNA based identification is not a new concept for other applications it has not been applied to pollen samples because pollen has been reported to not have enough chloroplast DNA for DNA barcoding and because sequence reads were too short and sequencing error rates too high. ARO support for research by Dr. Berry Brosi has demonstrated that DNA metabarcoding is a feasible approach for developing automated real-time pollen analysis. Professor Brosi published his latest results in FY17.[12] This work builds on prior ARO-funded, published work in the Brosi laboratory in collaboration with Army scientists from the Defense Forensic Science Center.[13]

F. Detection and Counting of Coliform Bacteria and Escherichia coli Via On-chip Imaging System

Investigator: Professor Aydogan Ozcan, University of California - Los Angeles, Single Investigator Award
Recipient: US Army Center for Environmental Health Research (USACEHR)

To protect the Warfighter from potential hazards posed from contaminated drinking water, the US Army Medical Research and Materiel Command (MRMC) has stated a need for a coliform analyzer for the detection of coliform bacteria and *Escherichia coli* in field drinking water supplies. Addressing this need, the U.S. Army Center for Environmental Health Research (USACEHR) sought technology to improve upon field tests currently used by U.S. Army preventive medicine personnel to better meet coliform analyzer requirements in terms speed, sensitivity of detection, portability and low cost.

USACEHR was made aware of the lens-free holographic cellular imaging technology developed by Professor Ozcan, with support through the ARO Life Sciences Division, as a potential engineered platform to meet these needs. In this microscopy-based platform, a diffraction pattern resulting from an object is recorded directly on a digital image sensor array without optical imaging or magnification by any lens elements. This recorded diffraction pattern is then computationally reconstructed to form an image of the object. Compared to lens-based microscopy, this technique allows for simultaneous large fields-of-view and high resolution as well as depth-resolved 3D imaging.

This research transitioned to USACEHR in FY17, which began providing funds to Professor Ozcan for a 3-year $593K effort to adapt and engineer a lens-free microscopy system. This system will be integrated with custom-designed machine learning algorithms to provide a compact, field portable, cost-effective imaging platform for automated detection, classification and counting of these bacterial contaminants. Efforts into FY18 include analysis of the bacterial growth on a filter membrane to reveal hyperspectral lens-free diffraction properties of each bacterial colony and the development and design of a graphical user interface (GUI) to control the entire lens-free coliform monitoring system.

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[12] Bell KL, Fowler J, Burgess KS, Dobbs EK, Gruenewald D, Lawley B, Morozumi C, Brosi BJ. (2017). Applying pollen DNA metabarcoding to the study of plant-pollinator interactions. *Appl Plant Sci.* 12:1600124.

[13] Bell KL, Burgess KS, Okamoto KC, Aranda R, Brosi BJ. (2016)/ Review and future prospects for DNA barcoding methods in forensic palynology. *Forensic Sci Int Genet.* 21:110-116.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Investigation of the Molecular Architecture of Spider Silk Protein Assembly

Professor Hannes Neuweiler, University of Wuerzburg, Germany, Single Investigator Award

Orb-web spiders use up to seven specialized glands to spin silk threads of different mechanical properties tailored for various tasks including prey capture, reproduction, and shelter. Silk from the major ampullate (Ma) gland, so-called dragline silk, is used to build the web frame or a lifeline (see FIGURE 12). Dragline silk is the toughest silk fiber and outperforms mechanical properties of man-made high-tech threads. Scientist have tried to reproduce the light-weight, protein-based material in the laboratory but with limited success. The main building blocks of the fiber are protein monomers, termed spidroins, of ~300 kDa molecular weight. Spidroins share a common, modular sequence architecture irrespective of species and gland, with a large, central segment consisting of repetitive peptide motifs that is flanked by non-repetitive amino- and carboxy-terminal domains (NTD and CTD, respectively). The goal of Professor Neuweiler's research is to reveal the assembly architecture and global conformation of spidroins in dragline silk, nature's toughest fiber, using the latest fluorescence spectroscopy and imaging methods with high temporal and spatial resolution.

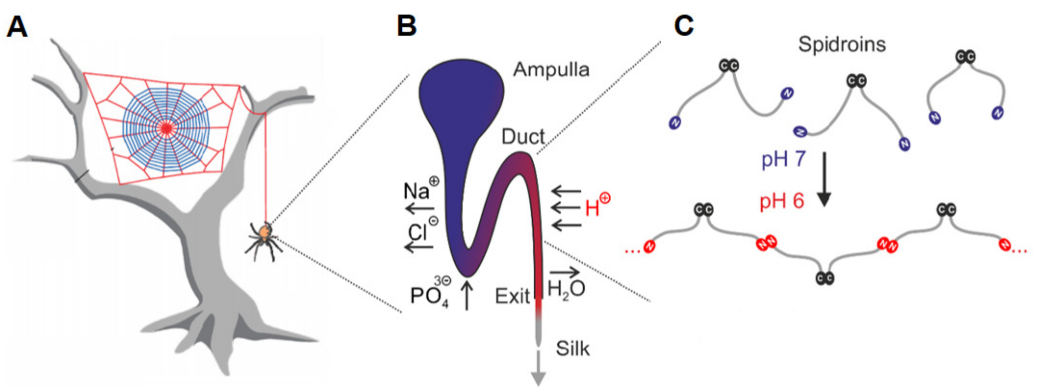

FIGURE 12

Synthesis of silk fibers by web spiders. (**A**) Silk from the major ampullate glad is used to build the web frame or a lifeline (red). (**B**) Schematic of a spider's spinneret. During silk synthesis spidroins pass from the ampulla of the gland through a tapering S-shaped duct where they experience a series of mechanical and chemical stimuli including shear forces, changes in salt composition and pH, before they leave the exit spigot as a solid silk fiber. (**C**) Schematic model of pH-triggered spidroin self-association facilitated by the NTD domain. The repetitive segments are shown as a grey line; NTD (N) and CTD (**C**) are indicated. Segments and domains are not to scale.

The NTD and CTD domains of spindroins are highly conserved, all-helical domains that provide water-solubility and facilitate assembly on demand using sophisticated mechanisms. Dragline silk mainly consists of two different types of spidroins, MaSp1 and MaSp2, which have different amino acid composition in their central segments. A highly concentrated solution of spidroins, called "dope", is stored in the ampulla of the spider's silk gland. The dope passes through a narrowing duct where spidroins undergo controlled phase and structural transitions before they leave the exit spigot as a solid fiber. On their journey through the duct they experience a series of mechanical and chemical stimuli. The dope is a non-Newtonian fluid that has special viscid properties. Shear forces are thought to align spidroins and changes of salt composition and pH induce structural transitions. The central segments are largely disordered in solution but form regular and non-regular secondary structural elements, mainly beta-sheets, in solid fibers. The conserved terminal domains play special roles in fiber formation besides providing solubility. The CTD is a homo-dimer, which is stabilized by a disulfide linkage, and connects two spidroin molecules covalently. A change of solution ionic strength appears to change the CTD structure, influencing assembly in the spinning duct. The NTD, on the other hand, contains a pH-sensitive switch. It is a monomer under storage conditions at pH 7 and forms a dimer at pH 5-6. A decreasing gradient of pH from 7 to 5.5 downstream from the spinning duct has been measured in dissected spider silk glands using staining and microelectrodes. pH-triggered self-association of NTDs might facilitate spidroin polymerization during their passage through the acidified assembly zone at the end of the spinning duct.

It is anticipated that in FY18 the research team will synthesize truncated black widow *Latrodectus hesperus* MaSp1 and MaSp2 sequences, consisting of central segments of 10 characteristic repetitive poly-alanine repeats flanked by the respective NTD and CTD. These sequences will be expressed in E. coli bacterial cells and purified using chromatographic methods for downstream fluorescence modification for imaging studies that will occur later in the project. The team will also adapt a dedicated fluorescence microscope for two-color imaging of spider silk.

The outcomes of this project will aid material scientists in tailoring and improving the strength and toughness of spider silk protein-based materials. Results are expected to provide hitherto unseen molecular-level structural information of spidroin interactions in silk and their dependence on external mechanical and chemical stimuli as they occur in an artificial spider's spinning duct. Knowledge gained as an outcome of this project will thus enable the refined design, optimization, and tailoring of mechanical properties of spider silk-based biomimetic material. The design and synthesis of new materials characterized by outstanding strength and toughness will provide new capabilities for Warfighter protection and performance. Spider silk is a current focus because it combines strength with elasticity yielding extreme toughness. At the same time, the protein-based fiber is biocompatible. Biocompatibility suggests applications not only where lightweight and tough material is required, such as protective clothing, body armor, parachutes, ropes and helmets, but also in the medical area for wound covers, artificial tendons and implants.

B. The Role of ApoE in Traumatic Brain Injury (TBI)

Professor Eric Schon, Columbia University, Single Investigator Award

The goal of this research is to determine how ApoE4 upregulates mitochondria-associated endoplasmic reticulum membranes. The investigators compared ApoE4 vs ApoE3 effects on mitochondria-associated endoplasmic reticulum membrane function following both pharmacological and genetic perturbations of candidate proteins involved in cholesterol homeostasis. They also used comparative transcriptomics and lipidomics to identify pathways that are differently affected by ApoE4 vs ApoE3. It is anticipated that in FY18, the team will determine whether cholesterol homeostasis plays a role in the ApoE4-mediated upregulation of mitochondria-associated endoplasmic reticulum membrane function. In addition, they hypothesize that ApoE may also affect mitochondria-associated endoplasmic reticulum membrane via pathways that are unrelated to cholesterol homeostasis. The transcriptomic and lipidomics experiments should reveal other pathways that affect mitochondria-associated endoplasmic reticulum membranes. This work led to the startling hypothesis that TBI may be mechanistically related to Alzheimer's disease. Humans with the (not uncommon) ApoE4 genetic variant have poorer outcomes after TBI than those with ApoE3. Further work is ongoing that, if successful, may lead to new therapeutics and prophylactics for both traumatic brain injury and Alzheimer's disease.

C. Imaging How a Neuron Computes

Professor Wei Min, Columbia University, MURI Award

There is a general lack of imaging tools available to visualize activity across the hundreds to thousands of synapses on a living neuron in a behaving brain. Fluorescence microscopy is the method of choice for live-cell imaging, but limitations prevent imaging more than 2-5 different molecules with high selectivity and sensitivity under biological conditions. One objective of this research project was to advance a special chemical imaging technique called Raman scattering to overcome these limitations. Raman scattering allows imaging of the vibrations from individual chemical bonds. However, previous advances have improved the technique but limited the potential for applying it in biological systems.

This MURI research effort sought to take the Stimulated Raman Scattering technique, developed by the leading PI of this work about a decade ago as a postdoctoral fellow at Harvard, and enhance the capability by making contributions from advances in spectroscopy and chemistry to create orders-of-magnitude more sensitive and mutually resolved vibrational 'tags' for labeling a large number of biomolecules at a time. The current research effort sought to test basic hypotheses about the chemistry underlying these vibrational tags, create a new library of probes and make proof-of-principle observations utilizing these new probes for understanding the intricate biological environment and activities of living tissues. In FY17, the researchers were able to demonstrate that fine-tuning this mode of chemical imaging along with developing superior chemical tags resulted in superbly sensitive and specific imaging of a large number of molecular species in live or fixed systems (see FIGURE 13). It was estimated that the newly developed tools offer about 1,000 times more sensitivity than the previous record for stimulated Raman scattering imaging and is demonstrated to show sensitivity comparable to that of confocal fluorescence microscopy.

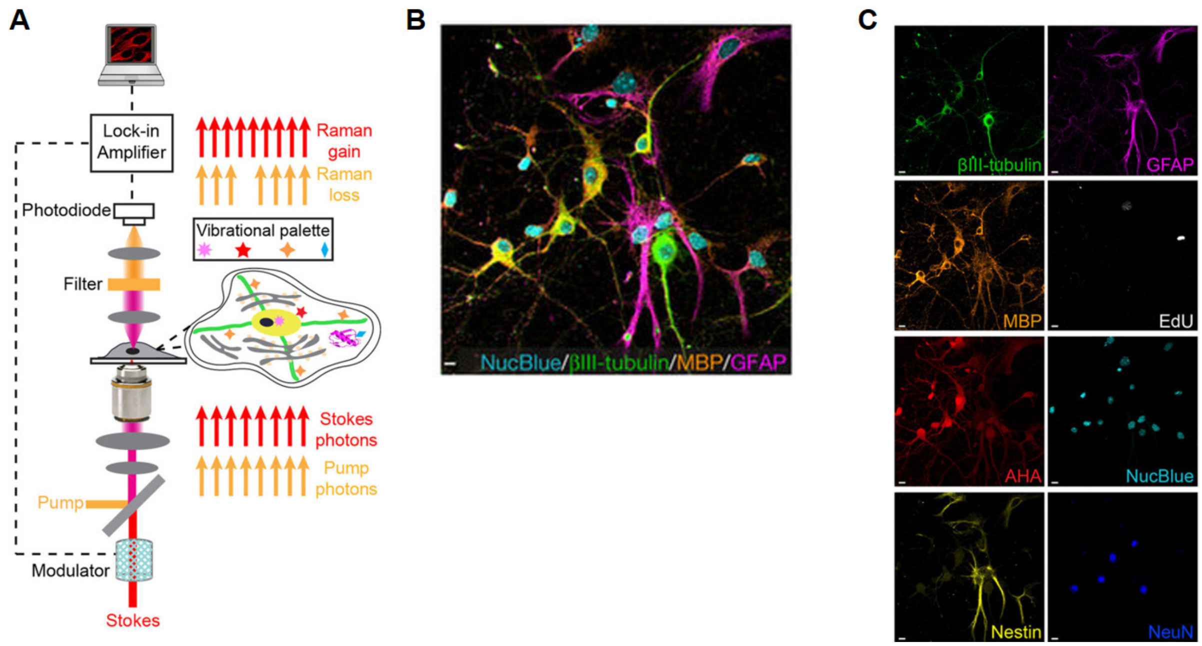

FIGURE 13

Super-multiplex optical microscopy and its applications for probing metabolic activity in nervous systems under physiological conditions. (**A**) A narrow-band pump laser and an intensity-modulated Stokes laser are synchronized before focusing the beams onto cell samples. When the energy difference between the pump photons and the Stokes photons matches the vibrational frequency (ω_{vib}) of the targeted chemical bonds, the chemical bonds are efficiently excited to the vibrational excited state. For each transition, a photon in the pump beam is annihilated (stimulated Raman loss) and a photon in the Stokes beam is created (stimulated Raman gain). A lock-in detection scheme is used to sensitively measure the intensity loss of the pump beam (that is, stimulated Raman loss). (**B**) Overlaid and (**C**) non-overlaid images of eight-colour epr-SRS imaging of DNA replication and protein synthesis in hippocampal neuronal cultures.

In FY18 it is anticipated that Professor Min's team will continue coupling advances in stimulated Raman scattering microscopy with other newly designed and synthesized vibrational probes (light-absorbing chromophores containing nitriles, alkynes or stable isotopes) to achieve more enhanced detection sensitivity and multiplexity. Effort will be focused on validating the exquisite vibrational selectivity of these new probes in biological samples thus allowing for a previously unachievable high number of colors that could be simultaneously imaged. The investigator is expected to continue validation experiments in living brain tissue in addition to creating new probes.

D. Forecasting Emergent Phenomena with Human-Computer Collaboration

Professor Boleslaw Szymanski, Rensselaer Polytechnic Institute, Single Investigator Award

The goal of this project is to generate new methods to identify threat networks. Professor Szymanski proposes that threats are interconnected, such that when a threat materializes, it may have either exacerbating or dampening effects on other threats in the network. For example, conflict within one community may spillover to another, or it may actually prevent conflict in the other community. Threats also vary with regard to their likelihood of materializing and with their likelihood of spilling over to other locations in the network. Moreover, networks have increasing geographical reach due to the growth in social media and other technologies that enable rapid and broad dissemination of information and events. Consequently, trying to predict threat risks and spillover has become a growing challenge and there is currently a lack of adequate theoretical and computational approaches.

Professor Szymanski is overcoming this limitation by integrating prospect theory, which identifies critical limits in the rationality of individual human decision-makers, with a novel crowdsourcing approaches to overcome those limitations, generating a mixed human-machine approach to threat detection, drawing on the World Economic Forum's data that identify of phenomena that pose economic, environmental, geopolitical, societal, and technological material threats. This approach takes human judgment and knowledge or threat as a starting point using crowd-sourced methods to develop the model. The crowd-sourcing approach enables thousands of estimations of threat risks and offers the potential to cancel individual biases which are randomly distributed throughout a population (see FIGURE 14). Computers then provide rapid empirical feedback to minimize speculation and generate more realistic models. Not only is Professor Szymanski's research generating new insights on human biases in judgmental decision-making and the distributions of those biases across a population, it is also enabling new capabilities for discovering hidden patterns in complex data that may contribution to those biases. Importantly, it has the potential to predict ripple effects and track the spillover of an error in one region of a network of complex interdependencies to other regions.

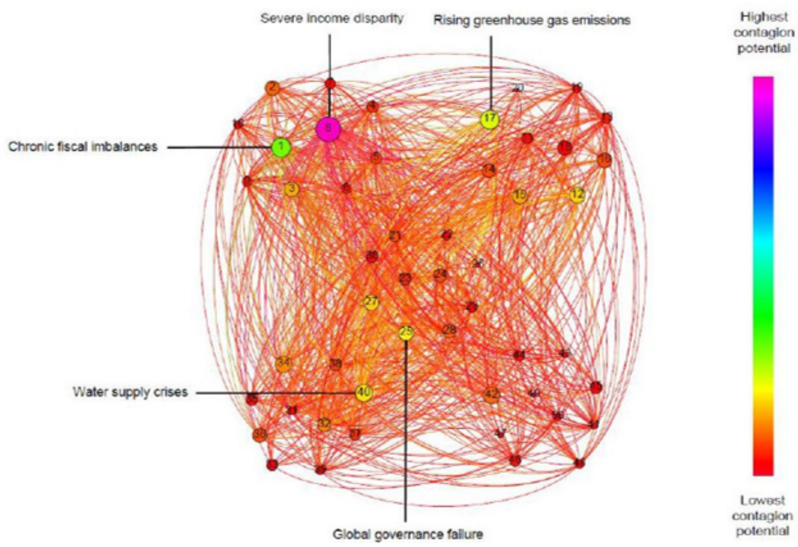

FIGURE 14

Global risk network derived from optimal model parameters. In this risk network, each node size is proportional the failure probability of the mechanism and the edges represent linkages between the mechanisms. Node color corresponds to the potential of the mechanism to adversely impact other mechanisms. This shows that the internal failure probability does not strictly generate a positive correlation with contagion over the network, suggesting that heightened risk does not necessarily inflict the most harm to the system.

The project offers the potential to rapidly develop risk models for different complex systems through crowd-sourcing while reducing bias in judgments, and offering visualization tools to quickly pinpoint critical regions with the greatest potential to generate system-wide failures. Professor Szymanski's work is also generating new insights on human-machine interaction to facilitate determinations of the balance between humans and computers in a wide range of judgmental decision-making contexts to improve performance by forecasting likely failure points, allowing for early intervention to avoid systemic crises.

E. Computational Models of Cultural Meaning & Social Interaction

Professor Dawn Robinson, University of Georgia, Single Investigator Award

The objective of this research is to develop computational models that capture culture and enable automated simulation of cross-cultural interaction by leveraging a large cross-cultural database. Cross-cultural understanding is essential to effective decision-making in the global contexts in which the U.S. Army operates. Yet, most cultural norms are not codified are often enacted without conscious consideration of the implications. Consequently, the state-of- the-art has been to train selected leaders and soldiers on the nuances of particular cultures or embed cultural experts in units working in particular regions of the world. Both of these strategies have proven costly and often ineffective. It is not plausible in rapidly changing environments to acquire the needed expertise that is only achieved through immersive experience in a culture and language fluency.

To overcome these barriers, this research project aims to develop computational models that can capture cultural norms, identities, activities and, importantly, the with-culture meanings of those activities to enable simulation of how interactions will unfold among actors from different cultures (that differ in one or more of the dimensions of meaning). The models will capture whether interaction will proceed smoothly and collaboratively, or lead to cross-cultural conflict, even when such conflict is not intended by either actor. Cultural competence is critical to effective decision-making in the dynamic and diverse environments in which military operations are carried out. Failure to recognize cross-cultural differences can lead to communication failures and the unintended escalation of conflict, but achieving cultural mastery has traditionally required intensive and extended immersion in the language and practices of the group, which is not always plausible when events are rapidly developing and involve multiple diverse groups.

Professor Robinson's laboratory is developing a compelling new approach through Affect Control Theory (ACT) to mathematically model meanings assigned to identities and actions in different cultures, enabling the ability to simulate and predict how interaction will unfold. In this approach the actors and behaviors are mathematically modeled in three dimensions of meaning (power, morality, and activity), which Robinson has demonstrated can be rapidly estimated for thousands of actors and behaviors in any cultural group using crowdsourcing approaches. Robinson has also developed equations to represent cultural rules for interaction, which predict the likelihood of combinations of actors and actions based on the degree to which the three dimensions of meaning for the actor and actions correspond. When correspondence is low, actors experience negative affect, which captures perceptions of disrespect or deviance on the part of the other actor. When actors detect such deviance it leads them to change their behavior to restore disrupted interaction. These changes occur with little conscious effort and make sense among members of the same culture who share meaning and the same rules for interactions. Because meanings and interaction rules are culturally dependent, however, when actors come from different cultures the lack awareness of the different rules and meanings governing each party's behavior can create unintended disruptions that spiral into unrepairable conflict, unpredictability, and volatile or even violent responses. Data from over a dozen cultures has been collected and the computational models capturing over 20 million interaction episodes are being developed. These models will become the basis for automated methods and tools to simulate cross-cultural interactions enabling greater capacity to generate on-the-fly analyses of the most effective interaction strategies in cross-cultural environments to achieve mission objectives.

F. Phenazine-mediated Extracellular Electron Transfer and Microbial Community Organization

Professor Dianne Newman, California Institute of Technology, Single Investigator Award

In their native environment, microorganisms are frequently organized in densely packed, spatially-static aggregates or "biofilms" where the biofilm composition ranges from populations of single species to communities of many phyla. The spatial organization of cells in biofilms is fixed by an extracellular matrix consisting of a number of bio-polymers (polysaccharides, proteins, nucleic acids) that consist of the contents of lysed cells as the biofilm is formed. A long-standing question has been whether this matrix plays an extended functional role within the biofilm aside from its mechanical role as a "glue"; that is, do the biochemical components of the matrix impart a metabolic advantage to the cells in the biofilm.

The Newman lab has explored the role of extracellular DNA (eDNA) within biofilms of the bacterium *Pseudomonas aeruginosa* (Pa) while addressing the question of how cells within the oxygen-depleted interior of the biofilm rise to the challenge of generating energy to survive. One important strategy that bacteria uses to meet this challenge is to produce extracellular electron shuttles. In Pa, redox-active molecules called phenazines are generated within biofilm cells, transported outside the cell where they are oxidized and then taken back up and re-reduced. Toward an understanding of how phenazines mediate extracellular electron transfer through Pa biofilms, Newman hypothesizes that eDNA may act as a substrate within the biofilm matrix for ordered phenazine binding and thus allow retention of these redox active molecules in the biofilm. Indeed, *in vitro* experiments have demonstrated that different phenazines bind DNA with different affinities and that those phenazines with higher affinity DNA binding show greater retention within the biofilm. In collaboration with Dr. Lenny Tender of the Naval Research Laboratory, Newman has also demonstrated that the rate of charge transfer through a Pa biofilm is consistent with an electron hopping model (vs a model relying on diffusion of the phenazines through the biofilm) which relies on close spatial deposition of these redox-active molecules (see FIGURE 15). Collectively, these results suggest that eDNA plays a role as a scaffold for phenazine binding and deposition within a biofilm allowing for efficient electron transfer and thus enabling cellular metabolism within the anoxic region of the biofilm.

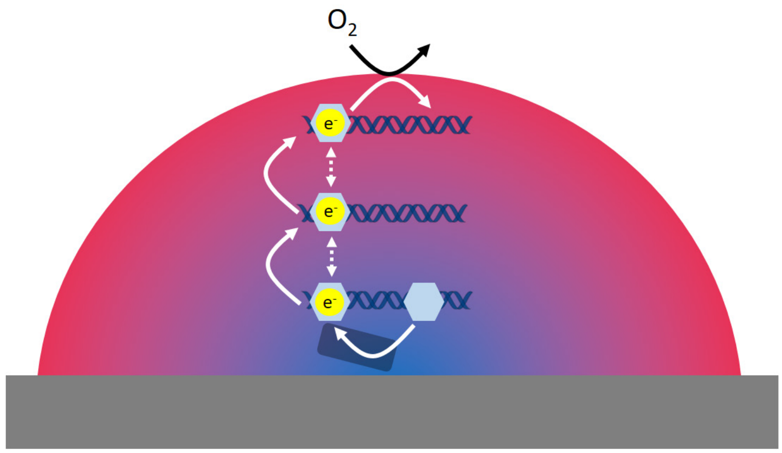

FIGURE 15

***P. aeruginosa* biofilm formed on a surface**. Zones of differing oxygen content (high-to-low O_2) are indicated by the red-to-blue transition. Initial data from Newman lab hypothesizes that electron transfer through the biofilm proceeds through a hopping mechanism affected by eDNA-bound phenazines (hexagons). The eDNA binding allows for enhanced phenazine retention and ordered phenazine deposition in the biofilm.

To further substantiate these findings, in FY18, the Newman lab will determine if eDNA is necessary and sufficient for phenazine retention in biofilms and for maintenance of charge transfer via electron hopping by repeating the above measurements after removing eDNA from the biofilm through DNase treatment, complementing with added eDNA and testing with cells that contain phenazine mutants. In addition synthetic phenazines will be tested for their electron hopping properties in biofilms and *in vitro*. For these experiments, techniques will be developed to optimize growth conditions for consistent biofilm thickness, the level of current generated within the biofilm will be titrated against phenazine concentration and conductivity measurements will be made with biofilms that have undergone drying to eliminate phenazine diffusion.

These experiments and insights will provide clues to how the biochemical components of the extracellular matrix may contribute to sustenance of biofilm activity and more generally, help build a foundation for a better understanding of how biofilms are formed and to inform the design of biofilm systems for a variety of applications including materials synthesis, bioremediation and electrosynthesis.

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A. Division Scientists

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CHAPTER 7: MATERIALS SCIENCE DIVISION

I. OVERVIEW

As described in *CHAPTER 1*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2017* is to provide an annual historical record summarizing the programs and basic research supported by ARO in FY17. ARO's mission is to support creative basic research resulting in new science that enables new materials, devices, processes, and capabilities for the current and future Soldier. This chapter provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions enabled by the ARO Materials Science Division in FY17.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Materials Science Division seeks to realize improved material properties by embracing long-term, high risk, high-payoff opportunities for the U.S. Army, with special emphasis on four Program Areas: Materials by Design, Mechanical Behavior of Materials, Physical Properties of Materials, and Synthesis and Processing of Materials. The objective of research supported by the Materials Science Division is to discover the fundamental relationships that link chemical composition, microstructure, and processing history with the resultant material properties and behavior. These research areas involve the discovery of the fundamental processes and structures found in nature, as well as developing new materials, material processes, and properties that promise to significantly improve the performance, increase the reliability, or reduce the cost of future Army systems. Fundamental research that lays the foundation for the design and manufacture of multicomponent systems such as composites, hierarchical materials and "smart materials" is of particular interest. Other areas of interest include new approaches for materials processing, composite formulations, and surface treatments that minimize environmental impact. Finally, there is general interest by the Division in research to identify and fund basic research in manufacturing science, which will address fundamental issues related to the reliability and cost (including environmental) associated with the production and long-term operation of Army systems.

2. Potential Applications. Research managed by the Materials Science Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter and battle systems. In the long term, the basic research discoveries made by ARO-supported materials research is expected to provide a broad base of disruptive and paradigm-shifting capabilities to address Army needs. Advanced materials will improve mobility, armaments, communications, personnel protection, and logistics support in the future. New materials will target previously identified Army needs for stronger, lightweight, durable, reliable, and less expensive materials and will provide the basis for future Army systems and devices. Breakthroughs will come as the fundamental understanding necessary to achieve multi-scale design of materials, control and engineering of defects, and integration of materials are developed.

3. Coordination with Other Divisions and Agencies. To realize the vision of the Materials Science Division and maximize transition and leveraging of new materials discoveries worldwide, the Division collaborates with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the Defense Advanced Research Projects Agency (DARPA), and across federal-funding agencies (*e.g.*, Nanoscale Science and Engineering Technology subcommittee, and in international forums (*e.g.*, the Technical Cooperation Program). The Materials Science Division is also very active in collaborating with other ARO Divisions to co-fund research, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. In particular, ongoing collaborations exist with the ARO Chemical Sciences, Electronics, Life Sciences, Mechanical Sciences, Mathematical Sciences, and Physics Divisions.

The Division's research portfolio will also reveal previously unexplored avenues for new Army capabilities while also providing results to support the ARL ERAs of (i) Impact of Operating in a Contested Environment, and (ii) Implementation. In addition, the Division supports the Materials Research Campaign's goals to extend the state-of-the-art in materials design, mechanical behavior of materials, physical properties of materials, and synthesis and processing research. The Division also supports the Sciences for Lethality and Protection Campaign with extraordinary lightweight materials, force-activated materials, stabilized nanostructured materials, manufacturing process science, novel electronics, and advanced sensory materials. The Division also supports the Sciences for Maneuver Campaign with unique materials for advanced power storage and generation and lightweight structures, in addition to low-cost manufacturing and repair processes.

B. Program Areas

The Materials Science Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY17, the Division managed research within these four Program Areas: (i) Materials by Design, (ii) Mechanical Behavior of Materials, (iii) Physical Properties of Materials, and (iv) Synthesis and Processing. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Materials by Design. The Materials by Design Program Area seeks to establish the experimental techniques and theoretical foundations needed to facilitate the hierarchical design and bottom-up assembly of multifunctional materials that will enable the implementation of advanced materials concepts including transformational optics, biomimetics and smart materials. This Program Area is divided into two research Thrusts:

(i) Directed 3D Self-Assembly of Materials is aimed at enabling the directed 3D assembly of reconfigurable materials, and developing viable approaches to the design and synthesis of multi-component materials incorporating hierarchical constructs.

(ii) Functional Integration of Materials focuses on demonstrating the predictive design and integration of functional properties into complex multi-component systems, and developing analytical techniques for interrogating the evolution of the 3D structure and properties of material assemblies at the nanoscale.

2. Mechanical Behavior of Materials. The Mechanical Behavior of Materials Program Area seeks to reveal underlying design principles and exploit emerging force-activated phenomena in a wide range of advanced materials to demonstrate unprecedented mechanical properties and complementary behaviors. This Program Area is divided into two research Thrusts:

(i) Force-Activated Materials involves demonstration and characterization of robust mechanochemically adaptive materials based on force-activated molecules and force-activated reactions, tailoring the deformation and failure mechanisms in materials to mitigate the propagation of intense stress-waves and control energy dissipation, and the creation of a new class of adaptive structural materials that demonstrate "mechanical homeostasis."

(ii) Mechanical Complements in Materials discovers superior ionic transport materials and transparent materials through a complementary, interdependent, optimization of mechanical properties, catalyzes a self-sustaining investigation of fiber precursors, tailored for lateral and axial interactions, to generate new paradigms for revolutionary structural fibers, and discovers and validates new atomic-scale strengthening mechanisms governing bulk mechanical behavior.

3. Physical Properties of Materials. The Physical Properties of Materials Program Area seeks to elucidate fundamental mechanisms responsible for achieving extraordinary electronic, photonic/optical, magnetic and thermal properties in advanced materials to enable innovative future Army applications. This Program Area is divided into two research Thrusts:

(i) Novel Functional Materials Thrust: This thrust supports the discovery of novel functional materials such as free-standing 2D materials/heterostructures/hybrids, Spin-Caloritronic materials, co-crystals, and other such materials with unique structures, compositions and properties. The thrust focus is on the synthesis, modeling and novel characterization of these materials (organic/inorganic/hybrids) to determine unprecedented functional properties (semiconducting, superconducting, ferroelectric/multiferroic etc.).

(ii) Defect Science & Engineering thrust explores the basic research opportunities in design, control and advanced characterization of various defects (point, line, area, volume etc.) in functional materials and elucidates different mechanisms during thin film growth/bulk materials processing that influence the extraordinary physical properties of functional materials.

4. Synthesis and Processing of Materials. The Synthesis and Processing of Materials Program Area seeks to discover and illuminate the governing processing-microstructure-property relationships for optimal creation of superior structural and bulk nanostructured materials. This Program Area is divided into two research Thrusts:

(i) Stability of Nanostructured Materials focuses on the creation of thermally-stable, ultrahigh strength nano-crystalline materials through interfacial grain boundary engineering, and the realization of high strength, stable nanostructured alloys via pinning nano-precipitates and internal coherent boundaries.

(ii) Manufacturing Process Science supports discovery of the fundamental physical laws and phenomena of materials processes, and the exploitation of unique phenomena that occur under metastable and complex processing conditions for the creation of revolutionary materials.

C. Research Investment

The total funds managed by the ARO Materials Science Division for FY17 were $42.8 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY17 ARO Core (BH57) program funding allotment for this Division was $9.7 million and $1.6 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $3.1 million to projects managed by the Division. The Division also managed $24.0 million of Defense Advanced Research Projects Agency (DARPA) programs, and $0.2 million provided by other Federal agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.1 million for contracts. In addition, $3.2 million was provided for awards in the Historically Black Colleges and Universities and Minority Serving Institutions (HBCU/MSI) Programs, including funding for DoD-funded Partnership in Research Transition (PIRT), DoD-funded Research and Educational Program (REP) projects, and $0.1 million of the Division's ARO Core (BH57) funds, with the latter included in the BH57 subtotal above.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY17 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY17 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY17, the Division awarded 26 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Jose Andrade, California Institute of Technology; *Grain Scale Interactions with Subterranean Structures: Material Removal Algorithms*
- Professor Jean-Luc Bredas, Georgia Tech Research Corporation; *Theoretical Description of Two-Dimensional Covalent Organic Frameworks (2D COFs)*
- Professor Mircea Dinca, Massachusetts Institute of Technology (MIT); *Physical Properties of Materials: Exotic Physical Properties of Electronically Coupled Two-Dimensional Metal-Organic Frameworks*
- Professor Bogdan Dragnea, Indiana University at Bloomington; *Materials Science. Optical Interactions in Bio-inspired Nanoparticle Systems*
- Professor Javier Garay, University of California - San Diego; *Research Area 9 Materials Science: Anistropic Microstructurally-engineered Polycrystals for increased Laser Engergy (AMPLE)*
- Professor Valery Levitas, Iowa State University of Science and Technology; *Phase transformation-related phenomena under compression and shear of ceramics*
- Professor Matthew Libera, Stevens Institute of Technology; *Multifunctional Antimicrobial Microgels*
- Professor Jonathan Malen, Carnegie Mellon University; *Physical Behavior of Layered Superatomic Crystals*
- Professor John Marohn, Cornell University; *Nanoscale Spin Hypepolarization and Imaging*
- Professor Thao (Vicky) Nguyen, Johns Hopkins University; *Extreme Dissipation Behavior of Main-Chain Liquid-Crystal Elastomers and Structures*
- Professor Corey O'Hearn, Yale University; *Strengthening and Armoring of Sheared Granular Beds*
- Professor David Pine, New York University; *Self-Assembly of Colloidal Diamond and Related Lattices for 3-D Photonic Band Gap Materials*
- Professor David Richter, University of Notre Dame; *Dust, sand, and turbulence: Transport and feedback in the near-surface environment*

- Professor Thomas Russell, University of Massachusetts - Amherst; *Liquid Tubules by the Self-Assembly of Self-Regulating NP Surfactants - Area 9.1 Materials by Design*
- Professor Richard Saykally, University of California - Berkeley; *Laser Spectoscopy of Liquid Carbon, Q-Carbon, and Their Surfaces; Application to Material Science*
- Professor Inanc Senocak, University of Pittsburgh; *Computational Modeling of Fundamental Exchange Processes from Heterogeneous Surfaces over Arbitrarily Complex Terrain*
- Professor Daniel Shoemaker, University of Illinois - Urbana - Champaign; *Synthesis and Processing of Materials: In Situ Scattering and Spectroscopy during Flash Sintering*
- Professor Douglas Spearot, University of Florida - Gainesville; *Virtual Diffraction Techniques used to Study Dislocation Loop ? Grain Boundary Interactions and Assess Slip Transfer Criteria*
- Professor Eli Sutter, University of Nebraska; *In-Situ Electron Microscopy of DNA-Guided Self-Assembly and Reconfiguration of 3D Nanocrystal Superlattices*
- Professor Izabela Szlufarska, University of Wisconsin - Madison; *Design of nanocrystalline alloys with superior wear resistance: Multiscale simulations and experiments*
- Professor Gregory Thompson, University of Alabama - Tuscaloosa; *Ascertaining the Thermo-Mechanical Mechanisms of Solute-Stabilized Nanocrystalline Alloys*
- Professor Norman Tolk, Vanderbilt University; *Depth-Dependent Transient and Permanent Materials Modification Arising from Ultrafast Laser Induced Carrier and Phonon Excitations*
- Professor Rodney Trice, Purdue University; *Forming Transparent Ceramics via Alignment of Alpha-Al2O3 Platelets: A Fundamental Investigation and Forming Study*
- Professor Harry Tuller, Massachusetts Institute of Technology (MIT); *Improved Ceramic Manufacturability With Electric Field Assisted Sintering: Developing Underlying Principles*
- Professor Yue Wu, University of North Carolina - Chapel Hill; *Thermodynamics and Dynamics of Metallic Liquids Studied by NMR: Liquid-Liquid Transition and Dynamic Crossover*
- Professor Brian Yanites, Indiana University at Bloomington; *Quantifying Rock Strength from River Channel Morphology*

2. Short Term Innovative Research (STIR) Program. In FY17, the Division awarded 11 new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Michel Barsoum, Drexel University; *On the Development of Polymer/MXene Composites*
- Professor Ricardo Castro, University of California - Davis; *W911NF-12-R-0012-03: Grain Boundary Polarization to Increase Toughness of Nanocrystalline Transparent Spinel*
- Professor Zachary Cordero, William Marsh Rice University; *Ultrasonic compaction of nanostructured powders*
- Professor Saptarshi Das, Pennsylvania State University; *Excitonic Devices based on 2D Heterostructures for Room Temperature Superconductivity*
- Professor William Fahrenholtz, Missouri University of Science and Technology; *Detonation Synthesis of Nanomaterials*
- Professor Olivia Graeve, University of California - San Diego; *Research Area 11.1 Short-Term Innovative Research (STIR) Program: Tailored Carbide Morphologies: Materials by Design for Creep Resistance at Ultra-high Temperatures*
- Professor Matthew Liberatore, University of Toledo; *Scalable, single step melt processing of anion exchange membranes*
- Professor Sefaattin Tongay, Arizona State University; *Alloys of Transition Metal Trichalcogenides for New-class of Two-dimensional Materials with Infrared Bandgaps*
- Professor Randy Vander Wal, Pennsylvania State University; *Engineering Nano/Micro Structure in C-C Composites by Templating*
- Professor Chengying Xu, Florida State University; *Effect of Pyrolysis Temperature on Electrical Properties and Conduction Mechanism of Polymer-Derived SiC Ceramics*

- Professor Yuntian Zhu, North Carolina State University; *Processing Heterogeneous Lamella fcc Alloys for Unprecedented High Strength and Ductility*

3. Young Investigator Program (YIP). In FY17, the Division awarded two new YIP projects to drive fundamental research in an area relevant to the current and future Army. The following PIs and corresponding organization_ was_ a recipient of the new-start YIP award.

- Professor Jason Kawasaki, University of Wisconsin - Madison; *Discovering new mechanisms for ferroelectricity in hexagonal half Heuslers*
- Professor Katherine Mirica, Dartmouth College; *Magnetoelectronic Sensors for Gasotransmitters*

4. Conferences, Workshops, and Symposia Support Program. The Division provided funds in support of a range of scientific conferences, workshops, and symposia that were held in FY17. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences, with the goal of supporting scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army, and to define the research needs, thrusts, opportunities, and innovation crucial to the future Army. Proposals requesting funding support, typically for less than $10K, were received and evaluated in line with the publicly available ARO BAA. In FY17, eleven proposals were selected for funding by the Division to support FY17 conferences, workshops, or symposia.

5. Special Programs. In FY17, the Division also awarded nine new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school and undergraduate students. These efforts were funded through the ARO Core Program and Youth Sciences Programs, for research to be performed at academic laboratories currently supported through active SI awards (refer to CHAPTER 2, Section IX).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Materials Science Division; therefore, all of the Division's active MURIs are described in this section.

1. Reconfigurable Matter from Programmable Colloids. This MURI began in FY10 and was granted to a team led by Professor Sharon Glotzer at the University of Michigan - Ann Arbor. This MURI project is co-managed by the Materials Science and the Chemical Sciences Divisions. The goal of this program is to enable the design and synthesis of an entirely new class of self-assembled, reconfigurable colloidal material capable of producing materials with radically increased complexity and functionality. This will revolutionize the ability to build complexity and functionality into materials in the future. Opportunities for manipulating the assembly process include the utilization of shape, intermolecular interactions, induced conformation changes, functionalized adduct and site-specific binding groups, molecule-to-substrate interactions, and external fields. Pathways including both sequential assembly and selective disassembly processes are being investigated. Selective disassembly and reconfigurability are to be accomplished by judicious exposure to heat, pH or light. The research includes aspects of self-limiting growth of superclusters. The experimental program is complemented by a very strong theoretical component. Research thrusts include:

- Sequential staged self-assembly of nano-particles into complex and hierarchical architectures
- Development of theoretical tools and computational algorithms to model the self-assembly process, to identify stable self-assembly pathways that lead to the targeted hierarchical structures, and finally to predict the final properties of the assembled material
- Future derivation of tailored properties and functions within highly complex or hierarchical materials

2. Stress-controlled Catalysis via Engineering Nanostructures. This MURI began in FY11 and was granted to a team led by Professor William Curtin at Brown University. The objective of this research is to prove that macroscopic applied loading can be used to actively control and tune catalytic reactions through the use of innovative nanoscale material systems.

This research is based on the hypothesis that active control using cyclically-applied stress can alleviate the well-established "volcano" effect wherein a desired reaction is optimal only in a narrow operating window due to competing reactions, and thereby overcome what has been believed to be a fundamental limiting factor in design of catalytic systems. The scientific underpinning will be demonstrated by developing two general platforms that can sustain high mechanical loading while also accommodating a range of material systems and catalytic reactions. The main outcome of the project will be the unambiguous proof-of-principle that stress can be used to substantially modify and control chemical reactions, along with possible engineering paths, via both thin film and bulk metallic glass nanostructures for implementing stress control across a wide material space.

3. Atomic Layers of Nitrides, Oxides, and Sulfides (ALNOS). This MURI began in FY11 and was granted to a team led by Professor Pulickel Ajayan at Rice University. The main objective of this MURI is to explore innovative top-down and bottom-up routes for the synthesis or isolation of high quality uni-lamellar sheets and ribbons of nitrides, oxides, and sulfides and to characterization these free standing 2D atomic layers to establish structure-property correlations in 2D layers.

The synthetic approaches of this research will span from simple mechanical/chemical exfoliation techniques to controlled chemical vapor deposition to create various 2D freestanding materials. Researchers will use computational tools based on density functional theory (DFT) methods to investigate binding energies, barriers and stabilities of different dopants and how they affect the band structure of the 2D host materials**.** 2D materials will be characterized for electrical conductivity/resistivity, Hall effect, carrier concentration, mobilities, ionic conductivity and thermal conductivity. If successful, this project could advance the basic science required to develop future DoD applications in chemical and biological sensors, opto-electronics, and power and energy.

4. Translating Biochemical Pathways to Non-Cellular Environment. This MURI began in FY12 and was awarded to a team led by Professor Hao Yan at Arizona State University. This research program is being co-managed by the Life Sciences and Materials Science Divisions. This MURI is exploring how biochemical pathways can potentially function in a non-cellular environment. Cells provide a precisely organized environment to promote maximum efficiency of biochemical reaction pathways, with individual enzymatic components organized via multi-subunit complexes, targeted localization in membranes, or specific interactions with scaffold proteins. The eventual translation of these complex pathways to engineered systems will require the ability to control and organize the individual components outside of the natural cellular environment. Although biological molecules have been successfully attached to inorganic materials, this process often requires chemical modification of the molecule and can restrict its conformational freedom. An alternative approach to maintain biological activity outside of the cell, while preserving conformational freedom, is to encapsulate enzymes within specialized materials or structures. Unfortunately, surface patterning of current encapsulating agents has not achieved the precision required to replicate the organizational capabilities of the cell.

The objective of this research is to develop the scientific foundations needed to design, assemble, and analyze biochemical pathways translated to a non-cellular environment using 3D DNA nanostructures. The MURI team is using DNA nanostructures to direct the assembly of selected biochemical pathways in non-cellular environments. The focus of this research is to develop the scientific foundations needed to translate multienzyme biochemical reaction pathways from the cellular environment to non-biological materials. The ability to translate biochemical reaction pathways to non-cellular environments is critical for the successful implementation of these pathways in DoD-relevant technologies including responsive material systems, solar cells, sensor technologies, and biomanufacturing processes.

5. The Physics of Surface States with Interactions Mediated by Bulk Properties, Defects and Surface Chemistry. This MURI began in FY12 and was awarded to a team led by Professor Robert Cava of Princeton University. This research is co-managed by the Physics and Materials Science Divisions. The objectives of this project are the discovery, growth, and fabrication of new materials that will display new topologically-stabilized electronic states in both 3D crystals and thin films grown by MBE. Those new materials will be characterized by many different methods including high resolution and spin resolved photoemission spectroscopy, transport, and STM measurements, X-ray scattering, and electron microscopy. The new materials of interest are particularly those that will display interactions arising from the presence of magnetism, such as those based on the heavy metal iridium, and interactions of topological states with superconductivity. State-of the- art materials science methods to optimize the properties of known topological insulators – in particular to enhance the interactions of the surface states with phenomena such as superconductivity are proposed. The correlation of the character of the chemically modified surfaces with the electronic properties will be performed. The team will address new frontiers in physics, such as proximity induced superconductivity in TIs, the 3D TI superconductor CuxBi2Se3, band bending surface capacitance and screening in TIs, and the giant Rashba effect in BiTeI etc.

6. Materials with Extraordinary Spin/Heat Coupling. This MURI began in FY13 and was granted to a team led by Professor Roberto Myers of Ohio State University. The objectives of this project include understanding the structure-property relationships for coupling heat and spin current in various materials and synthesize magnetic materials with extraordinary and tunable thermal conductivity due to spins, understanding non-equilibrium phonon-magnon transport and the mechanisms behind Spin Seebeck Effect, and finally measuring and understanding phonon-magnon drag and phonon-electron drag in materials.

If successful, this project may lead to long-term applications such as temperature sensors, thermal spintronic devices, solid-state Spin Seebeck Effect -based power generators, thermal management in electronic and vehicular applications, and tunable thermal conductivity in materials via magnetic field, microwaves, and light.

7. Theory and Experiment of Cocrystals: Principles, Synthesis and Properties. This MURI began in FY13 and was awarded to a team led by Professor Adam Matzger of the University of Michigan at Ann Arbor. This MURI team is investigating molecular co-crystal formation and the implications for controlling solid-state behavior. This research is co-managed by the Chemical Sciences and Materials Science Divisions.

The largely untapped potential for creating new molecular crystals with optimal properties is just beginning to be realized in the form of molecular co-crystallization. Co-crystallization has the potential to impact the macro-scale performance of many materials, ranging from energetic materials, to pharmaceuticals, to non-linear optics. Unfortunately, the dynamics of molecular co-crystal formation is poorly understood. Molecular co-crystals contain two or more neutral molecular components that rely on non-covalent interactions to form a regular arrangement in the solid state. Co-crystals are a unique form of matter, and are not simply the result of mixing two solid phases. Organic binary co-crystals are the simplest type and often display dramatically different physical properties when compared with the pure 'parent' crystals. A significant amount of research on co-crystal design has been carried out by the pharmaceutical industry for the synthesis of pharmaceutical ingredients. However, co-crystal design has not been exploited in broader chemistry and materials science research areas. A recent breakthrough discovery demonstrates that co-crystallization can be used to generate novel solid forms of energetic materials.

The objective of this MURI is to develop a fundamental understanding of intermolecular interactions in the context of crystal packing, and to use the knowledge gained for the design of new co-crystalline molecular materials with targeted, optimized physical and chemical properties. In the long term, a better understanding and control of molecular co-crystallization has the potential to improve the properties of a variety of materials, including: energetic materials, pharmaceuticals, organic semiconductors, ferroelectrics, and non-linear optical materials.

8. Multiscale Mathematical Modeling and Design Realization of Novel 2D Functional Materials. This MURI began in FY14 and was awarded to a team led by Professor Mitchell Luskin of the University of Minnesota. This research is co-managed by the Mathematics and Materials Science Divisions. The objective of this project is to develop efficient and reliable multiscale methods to couple atomistic scales to the mesoscopic and the macroscopic continuum for layered heterostructures. Layered heterostructures represent a dynamic new field of research that has emerged from recent advances in producing single atomic layers of semi-metals (graphene), insulators (boron nitride) and semiconductors (transition metal dichalcogenides). Combining the properties of these layers opens almost unlimited possibilities for novel devices with desirable, tailor-made electronic, optical, magnetic, thermal and mechanical properties. The vast range of possible choices requires theoretical and computational guidance of experimental searches; experimental discovery can in turn inform, refine and constrain the theoretical predictions.

The proposed research will develop efficient and reliable strongly-linked multiscale methods for coupling several scales based on a rigorous mathematical basis. Specifically: 1) The rigorous coupling of quantum to molecular mechanics will be achieved by properly taking into account the mathematics of aperiodic layered structures. 2) The coupling of atomistic-to-continuum will be achieved by methods that can reach the length scales necessary to include long-range elastic effects while accurately resolving defect cores. 3) New accelerated hybrid molecular simulation methods, specially tailored for the weakly interacting van der Waals heterostructures, will be developed that can reach the time scales necessary for synthesis and processing by CVD and MBE. 4) The simulations will be linked to macro and electromagnetic modelling to understand the physics and bridge to experimental investigation.

The challenge of modeling layered heterostructures will promote the development of strongly-linked multiscale models capable of handling many other materials systems with varied applications, including composites, meta-atoms (atomically engineered structures), and bio-materials that are of interest to the Army.

9. Advanced 2D Organic Networks. This MURI began in FY16 and was granted to a team led by Professor William Dichtel at Cornell University. The objective of this research is to create stable, free-standing, single-monomer-thick 2D crystalline organic polymer nanosheets/covalent organic frameworks (COFs) with designed electronic (conductivity, mobility, charge storage), optical (resonances, nonlinearities), and structural properties.

The team will combine mechanistic studies, theory, microscopy, and spectroscopy to gain fundamental insight into the 2D polymerization processes. Specifically the team will address the challenges in 2D COF synthesis and characterization by focusing on the following three major research thrusts: (1) exploration of nucleation, bond exchange, and polymerization of 2D COFs to improve their long-range order and morphological form and isolate 2D COFs as single crystals; (2) investigation of new conjugated linkage chemistries, topologies, and doping strategies to impart extensive electronic delocalization and useful optical and electronic properties; and (3) fabrication of new hybrid device heterostructures based on the interfacing of 2D COFs with newly emerging 2D inorganic materials such as transition metal dichalcogenides.

10. Specifically Triggerable Multi-Scale Responses in Organized Assemblies MURI. This MURI began in FY16 and was awarded to a team led by Professor Sankaran Thayumanavan of the University of Massachusetts – Amherst and is being jointly managed by the Materials Science and the Chemical Sciences Divisions. The goal of this effort is to develop a fundamental understanding of how a molecular level detection event can be amplified and then propagated across a macroscopic material to affect a global property change that spans multiple length and time scales. Fundamental approaches for converting single event triggers into extended material responses based on liquid crystal reorientation, regulated amphiphile assembly, gel-to-sol depolymerization and release reactions, and protein-induced transformations are being investigated. A variety of trigger mechanisms based on pH, temperature, redox, light, and enzymatic release are to be developed. A key aspect of this effort is the real-time monitoring of the dynamic changes associated with the cooperative reorganization processes combined with a strong theoretical component aimed at developing models of the material responses and corresponding phase behavior. The breadth of this effort allows for objectives to be pursued in parallel to achieve a fundamental understanding of multi-scale signal propagation and amplification in hierarchical systems and the development of rational design principles for fabricating dynamically responsive material systems.

11. Quantum Materials by Design with Electromagnetic Excitation. This MURI began in FY16 and was awarded to a team led by Prof David Hsieh of Caltech and is being jointly managed by the Physics and Materials Science Divisions. The objective of the project is to create new electronic states of matter that are unobtainable through conventional solid-state synthesis. The team proposes to employ excitations across the entire electromagnetic (EM) spectrum, including with extremely high pulsed fields, to design, realize, and manipulate new phases and responses in strongly correlated materials. Specifically, the team will focus on realizing new correlated states via the following approaches, (1) EM stimulated, bond selective, tuning of charge hopping parameters, (2) direct EM modification of magnetic exchange, order, and frustration, (3) continuous EM control of dimensionality and hybridization, and (4) EM excitation across kinetic barriers to realize metastable states that are thermodynamically inaccessible. Using these non-equilibrium methods, they will aim at realizing some of the most sought-after phenomena in condensed matter physics including collective charge/current ordered phases, bandwidth controlled metal to Mott insulator transitions, quantum disordered magnets such as valence bond solids and highly entangled quantum spin liquid states, and low dimensional and quantum critical electron liquids with no quasiparticle description.

12. Abelian Bridge to Non-Abelian Anyons in Ultra-Cold Atoms and Graphene. This MURI began in FY17 and was awarded to a team led by Professor Andrea Young of the University of California - Santa Barbara and is jointly managed by the Physics and Materials Science Divisions. This MURI aims to demonstrate and comprehensively explore nonabelian anyons via an interdependent investigation of solid-state materials and ultracold atoms. The MURI team proposes to develop three experimental avenues to nonabelian physics, focusing on the most promising cold-atom and solid-state candidates: realizing intrinsic nonabelian ground states, engineering synthetic nonabelian defects via Cooper pairing, and creating related defects by purely geometric means.

13. Adaptive Self-assembled Systems. This MURI began in FY17 and was awarded to a team led by Professor Anna Balazs of the University of Pittsburgh and is being jointly managed by the Materials Science and the Chemical Sciences Divisions. The goal of this effort is to develop experimental and theoretical approaches to integrate microscopic forms of self-organization with a scalable means of additive 3D fabrication.

This effort is organized around three major thrusts: (i) assembly of microscale musculoskeletal frameworks, (ii) transduction of energy to enable functionality, and (iii) additive manufacturing of large-scale dynamic material systems. If successful, the research will enable the development of artificial "smart" materials and structures that exhibit tightly coupled capabilities for sensing environmental cues and then transducing energy to perform useful, situation-specific dynamic responses.

C. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY17.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPSTIONS AND FUNDING SOURCES*. In FY17, the Division managed one new-start STTR contract, in addition to active projects continuing from prior years. This new-start contract aims to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY17 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Serving Institutions (HBCU/MSI) – New Starts

The HBCU/MSI program encompasses the (i) Partnership in Research Transition (PIRT) Program awards, (ii) DoD Research and Educational Program (REP) awards for HBCU/MSIs, and (iii) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY17, the Division managed three new REP awards, in addition to active projects continuing from prior years. In addition, proposals from HBCU/MSIs are often among the projects selected for funding by the Division (refer to the list of HBCU/MSI new starts in *CHAPTER 2, Section IX*.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY17.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY17, the Division managed 8 new DURIP projects, totaling $1.8 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. DARPA Nanostructured Materials for Power (NMP) Program

The DARPA NMP program seeks to exploit advanced nano-structured materials for revolutionary improvements in power applications of DoD interest. The ability to decouple and independently control physical, chemical, electromagnetic, and thermal phenomena through nanoscale design, is being tapped to enable improvements in the energy product of permanent magnets and the efficiency of future thermoelectric devices. The Materials Science Division currently co-manages projects within this program. The goals of these projects are ultimately to provide new nano-structured magnetic and thermoelectric materials with enhanced figures of merit for development of higher performance compact power sources in the future.

I. DARPA LoCo Program

The goal of the Local Control of Materials Synthesis (LoCo) program is to develop a low-temperature process for the deposition of thin films whose current minimum processing temperature exceeds the maximum temperature substrates of interest can withstand (e.g., chemical vapor deposited diamond on polymers). The Division currently co-manages projects within this program seeking to realize chemical and physical processes to meet the energetic/chemical requirements of thin film deposition (e.g., reactant flux, surface mobility, reaction energy, etc.), without reliance on broadband temperature input used in state-of-the-art chemical vapor deposition.

J. DARPA Low-Cost Light Weight Portable Photovoltaics (PoP) Program

The goal of the DARPA PoP program is to provide low-cost light-weight portable photovoltaics to DoD. The Materials Science Division currently co-manages projects within this program with the goal of exploring new materials solutions that can meet these goals.

K. DARPA Manufacturing Experimentation and Outreach (MENTOR2) Program

The DARPA MENTOR2 Program seeks to enhance defense readiness by improving both the training and the tools available to those who will be called on to utilize, maintain, and adapt high-technology systems in low-technology environments. MENTOR2 will pursue this goal by developing and demonstrating new training tools, new materials, and new manufacturing technologies in the fields of electromechanical design and manufacturing. It is envisioned that project based curricula employing MENTOR2 design and prototyping tools will teach a deeper understanding of high-technology systems and better enable future competence in the maintenance and adaptation of such systems through the manufacture of as-designed components or the design and manufacture of new components. The Division currently co-manages projects within this program seeking to explore the integration of materials manufacturing and learning approaches to develop and demonstrate new approaches to electromechanical design.

L. DARPA Maximum Mobility and Manipulation Program

The DARPA Maximum Mobility and Manipulation program seeks to create and demonstrate significant scientific and engineering advances in robotics that will create a significantly improved scientific framework for the rapid design and fabrication of robot systems and greatly enhance robot mobility and manipulation in natural environments. Additionally, the program seeks to significantly improve robot capabilities through fundamentally new approaches to the engineering of better design tools, fabrication methods, and control algorithms. The Maximum Mobility and Manipulation program covers scientific advancement across four tracks: design tools, fabrication methodologies, control methods, and technology demonstration prototypes. The Division currently co-manages projects within this program seeking to realize novel material design and fabrication paradigms for advanced sensing and actuation materials.

M. DARPA Microphysiological Systems Program

The DARPA Microphysiological Systems program seeks to develop a platform that uses engineered human tissue to mimic human physiological systems. The interactions that candidate drugs and vaccines have with these mimics will accurately predict the safety and effectiveness that the countermeasures would have if administered to humans. As a result, only safe and effective countermeasures will be fully developed for potential use in clinical trials while ineffective or toxic ones will be rejected early in the development process. The resulting platform should increase the quality and potentially the number of novel therapies that move through the pipeline and into clinical care. The Division currently co-manages projects within this program seeking to realize safe and effective countermeasures based upon novel characterization tools, molecular structures, and materials architectures.

N. High Energy Laser Research & Development for HEL-JTO

The High Energy Laser Research & Development Program seeks to support farsighted, high payoff scientific studies leading to advances in HEL science and technology science with the end goal of making HELs lightweight, affordable, supportable, and effective on the modern battlefield. The Division currently manages solid-state laser research of processes and technologies that provide enhancement to the manufacturability of current and innovative design of ceramic gain material.

O. DARPA Materials for Transduction (MATRIX), DSO-DARPA

Transducer materials convert energy from one form to another, such as thermal to electrical energy, or electric field to magnetic field. While significant progress has been made in advancing energy transducing material performance (e.g. thermoelectrics, multiferroics and phase changing materials) for certain applications, gains at the material level have not always translated into new devices and DoD capabilities. The goal of the MATRIX program is to extend materials breakthroughs to the device and systems level by integrating diverse modeling, design and fabrication communities in a unified research and development effort that bridges the material and the device domains. A major program thrust is the development of multiscale, multimodal design and engineering tools that have the potential to accelerate adoption of MATRIX technology into DoD platforms. The Division currently manages five programs within this DARPA Program:

- Solid State (Gyrator) Device for Low Power Electronics; Dwight Viehland, Virginia Tech.
- Phase-Change Materials Enabling Hyperspectral Imaging: Jeong Moon, HRL
- Wireless Cooling with Caloric Materials: Amy Duwel, Draper Labs
- Tunable Energy Efficient Multiferroic-based Electronics: Shashank Priya, Virginia Tech
- Integrated Magnetoelectric Devices: Carmine Vittoria, Northeastern University

P. DARPA Tailorable Feedstock and Forming Program

The DARPA Tailorable Feedstock and Forming program seeks to develop a new composite material format (i.e., feedstock) and associated processing technologies (e.g., reconfigurable forming) to reduce manufacturing complexity and enable use of advanced materials for small parts. The capabilities and technical specifications required for DoD platforms are constantly changing due to unanticipated circumstances, needs and emerging threats. However, complex development and design cycles and the associated high costs of structural design changes for current technologies significantly limit the ability to rapidly and affordably evolve such systems. The technologies envisioned by this program would enable greater efficiency in manufacturing advanced DoD small composite parts with decreased development and production costs. The Division currently co-manages projects within this program seeking to realize a flexible forming/molding manufacturing process to enable the fabrication of low-cost small composite structural parts.

Q. DARPA Hand Proprioception and Touch Interfaces

The DARPA Hand Proprioception and Touch Interfaces program is pursuing key technologies to enable precision control of and sensory feedback from sensor-equipped upper-limb prosthetic devices. If successful, the resulting system would provide users near-natural control of prosthetic hands and arms via bi-directional peripheral nerve implants. A key focus of HAPTIX is on creating new technologies to interface permanently and continuously with the peripheral nerves in humans. It is anticipated that a completed HAPTIX system will be integrated with one of the advanced prosthetic limbs developed under DARPA's Revolutionizing Prosthetics program to create the first dexterous prosthetic limb with full sensory and motor capabilities that is suitable for home use. The Division currently co-manages projects within this program seeking to explore and develop adaptive neural-enabled sensory feedback and stimulation approaches to enhance functionality and safety in revolutionary prosthetic systems.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Materials Science Division.

A. Physical Properties of Electronically Coupled Two-Dimensional Metal-Organic Frameworks

Professor Mircea Dinca, Massachusetts Institute of Technology, Single Investigator Award

The objective of this project is to study the fundamental properties of hybrid organic-inorganic materials known as metal-organic frameworks (MOF), particularly materials made from two-dimensional sheets stacked through Van der Waals interactions. This effort showed the first signature of metallic behavior in a MOF, Ni_3(hexaiminobenzene)$_2$, with a graphite-like structure (see FIGURE 1). The key experiment suggesting a metallic state was an ultraviolet photoelectron spectroscopy (UPS) measurement that revealed a continuum of electronic states (see FIGURE 2).

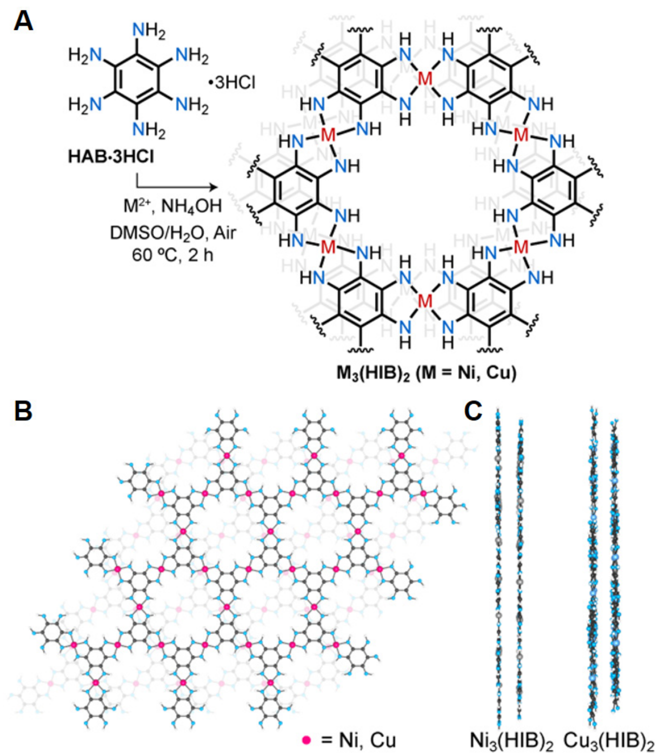

FIGURE 1

First signature of metallic behavior in a MOF, Ni_3(hexaiminobenzene)$_2$. (**A**) synthesis, (**B**) top view, and (**C**) side view of the structure.

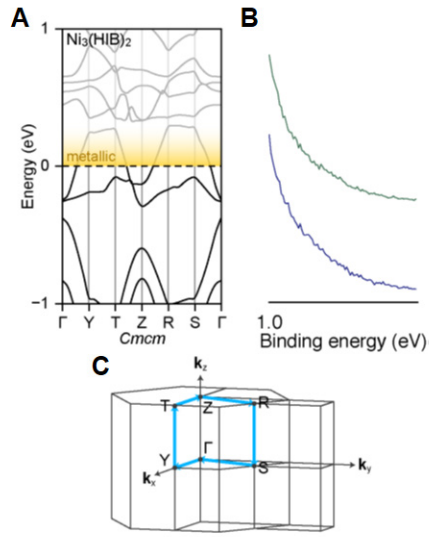

FIGURE 2

Ultraviolet photoelectron spectroscopy (UPS) measurement that revealed a continuum of electronic states. (A) computed band structure and (B) UPS for $Ni_3(HIB)_2$ The metallic state was predicted and is in agreement with the computed band structure of the material.

B. Two Dimensional Growth of Free-Standing Nanosheets and Heterostructures by Ionic Layer Epitaxy

Professor Xudong Wang, University of Wisconsin - Madison, Single Investigator Award

The objective of this research is to understand the nucleation and growth mechanisms of nanosheets of various materials at a water-air interface guided by surfactant monolayers and there by achieve a rational control over the thickness and the grain size of these nanosheets. In this effort a novel Ionic Layer Epitaxy (ILE) technique was developed, which is the first solution-based technique for growing large-area free-standing single crystalline ultrathin nanosheets without the support of crystalline substrates. ILE was first demonstrated by the growth of single crystal ZnO nanosheets at the water-air interface directed by a monolayer of amphiphilic molecules (see FIGURE 1). High-resolution transmission electron microscopy (HRTEM) revealed that the nanosheet was polycrystalline, which was different from the single crystal feature obtained from the water-air interface. Both single-crystalline and polycrystalline nanosheets exhibited a temperature-independent (5K to room temp.) ferromagnetism with a saturation magnetization of 35.3 and 54.2 emu g^{-1}, respectively. The surface defect-related magnetism of ZnO nanosheets was 3-5 orders of magnitude higher than other ZnO morphologies and as high as Fe_3O_4 owing to their ultrasmall thickness. ILE vastly broadens the range of 2D nanomaterials from layered van der Waals solids to oxides, ceramics, and metals, opening up opportunities for discoveries of exciting transport, photonic, and catalytic properties. In addition to ZnO, this effort showed successful synthesis results of single crystalline CoO, MnO_2, NiO with a thickness of one to a few unit-cells.

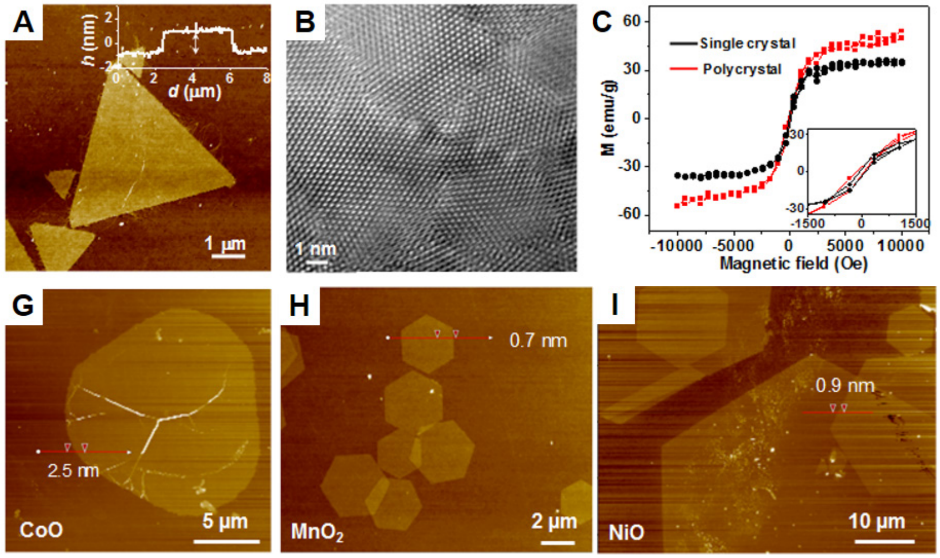

FIGURE 3

Demonstration of Ionic Layer Epitaxy (ILE) via growth of single crystal ZnO nanosheets at the water-air interface directed by a monolayer of amphiphilic molecules. (A) AFM image of ZnO nanosheets grown at water-toluene interface. (B) HRTEM image of the ZnO nanosheet showing a polycrystalline structure. High-resolution transmission electron microscopy (HRTEM) revealed that the nanosheet was polycrystalline, which was different from the single crystal feature obtained from the water-air interface. (C) Magnetic hysteresis curves measured from single-crystalline ZnO (black) and polycrystalline ZnO (red). Both single-crystalline and polycrystalline nanosheets exhibited a temperature-independent (5K to room temp.) ferromagnetism with a saturation magnetization of 35.3 and 54.2 emu g^{-1}, respectively. (G-J) AFM images of ultrathin single-crystalline nanosheets made from CoO, MnO_2, and NiO, respectively.

C. Self Assembly of Percolating Colloidal Structures Capable of Displaying Omnidirectional Photonic Bandgaps

Professor David Pine, New York University, MURI Award

Percolating "open" structures like diamond and pyrochlore lattices can afford unique optical properties (e.g., omnidirectional photonic bandgaps). However, they are almost impossible to prepare using self-assembly methods due to their low space filling factor (34 vol% vs 74 vol % for close packed spheres), which is unable to support the open structures. However, researchers at NYU have recognized that these open structures exist together as two interpenetrating sublattices within the close-packed $MgCu_2$ superlattice (see Figure 4). They have also showed that this structure can be prepared via DNA-mediated assembly, although it requires the preassembly of tetrahedral clusters (making up the pyrochlore phase) to drive the assembly towards formation of the desired pyrochlore phase. To date, the assembly of the $MgCu_2$ superlattice has been successfully demonstrated using a mixture of polystyrene (PS) particles and PS tetragonal clusters followed by a long anneal (several hours) at temperatures just below the melting point of the DNA assembly (46°C). The team is now exploring whether these structures will produce a photonic bandgap by creating a mixture of titania particles and polystyrene tetrahedral clusters, which would introduce a refractive index contrast greater than two between the two sublattices.

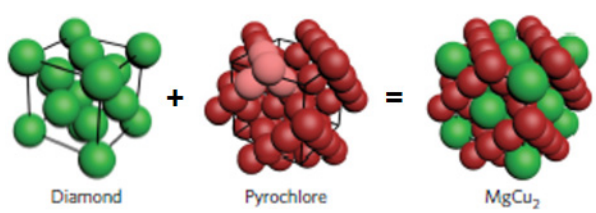

FIGURE 4

Open structures exist together as two interpenetrating sublattices within the close-packed $MgCu_2$ superlattice.

D. Biomimetic 4D Printing

Professor Jennifer Lewis, Harvard University, Single Investigator Award

The objective of this research is to fabricate temporally and spatially patterned gels and nanocomposites that undergo dramatic changes in chemo-mechanical properties in response to external stimuli. The research team has sought to control not only the spatial dimensions of the sample, but also the time-dependent behavior of the system and hence, to enable patterning in space and time. Furthermore, the work has designed new gel and nanocomposite inks that are stimuli-responsive and can be made to exhibit complex temporal behavior with changes in external cues. In FY17, the effort successfully fabricated unique composite hydrogel architectures that change shape when immersed in water, yielding first-ever complex three-dimensional morphologies that accurately mimic the structure and dynamics of botanical systems (see FIGURE 5). These novel hydrogel architectures are engineered with localized, anisotropic swelling behavior controlled by the alignment of cellulose fibrils along prescribed four-dimensional printing pathways. When combined with a basic algorithm to solve the inverse problem of designing the alignment patterns for prescribed target shapes, unique architectures that can be programmed to change shape in water can now be precisely and consistently fabricated. The hydrogel composite ink combines stiff cellulose fibrils in a soft acrylamide matrix, which is similar in structure to the composition of plant cell walls. The composite architectures are printed using a viscoelastic ink that contains N,N-dimethylacrylamide (or N-isopropylacrylamide for reversible systems), a photoinitiator, nanoclay, glucose oxidase, glucose, and nanofibrillated cellulose (NFC). The clay particles serve as a rheological aid, glucose oxidase and glucose minimize oxygen inhibition during ultraviolet curing for mechanically robust structures, and the cellulose fibrils provide additional stiffness to the structures. After printing under ambient conditions, the acrylamide monomer is photopolymerized and physically crosslinked by the nanoclay particles, producing a biocompatible hydrogel matrix that swells readily in water.

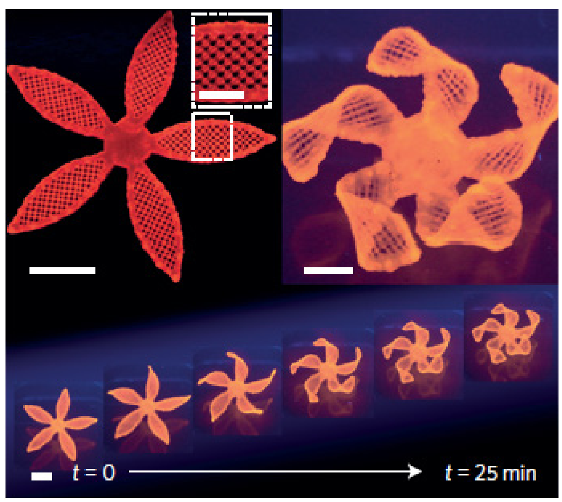

FIGURE 5

Complex flower morphologies generated by biomimetic 4D printing. The structure is comprised of bilayers oriented with respect to the long axis of each petal, with time-lapse sequences of the flowers during the swelling process. (Scale bars: 5 mm, inset = 2.5 mm).

E. Controlled Dispersion of Nanoparticles into 3D Patterns via Ultrasonic Dispersion

Professor Bart Raeymaekers, University of Utah, Single Investigator Award

The objective of this project is to enable the controlled creation of nanoparticle patterns in polymers and other viscous media using ultrasonic waves. The interaction of a particle's surface with an ultrasonic wave creates an acoustic radiation force that drives the particles to locations where the force is minimized. In FY17, the research team developed computational tools that predict the particle motion that results from these forces and used those tools to successfully create organized 3D patterns of carbon nanoparticles in poly(methyl methacrylate). This is the first demonstration of an organized 3D particle arrangement created by ultrasonic dispersion in a viscous medium (see FIGURE 6). It was found that the addition of a third dimension placed greater emphasis on near field effects and acoustic reflections that increased pattern error over 2D experiments. Nevertheless, strong agreement between the simulations and experimentally observed patterns was observed, and as the work progresses these sources of error are being addressed in the computational calculations. This accomplishment establishes that it is technically feasible to disperse a secondary phase into a matrix in a specific arrangement using ultrasonic waves and lays the technical foundation for an entirely new method of designing composite materials with unprecedented mechanical or electronic properties.

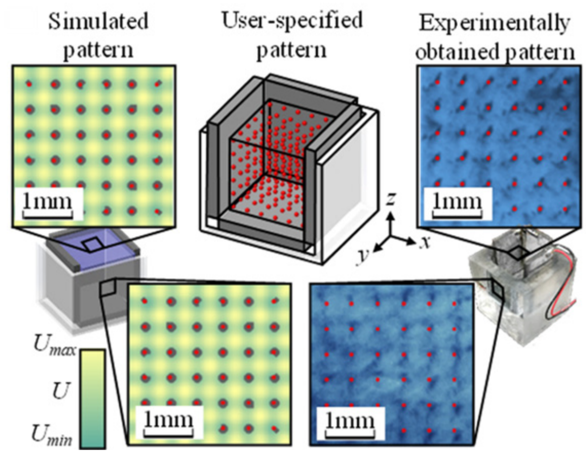

FIGURE 6

Three-dimensional pattern of carbon nanoparticles created via ultrasonic dispersion in a polymer medium.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Low Power Monolayer MoS_2 Transistors for RF Applications

Investigator: Dr. Rajesh Rao, Applied Novel Devices Inc., STTR Contract
Recipients: ARL-SEDD

The objective of this project is to demonstrate the feasibility of producing large area, single crystal monolayer Molybdenum disulfide (MoS_2) for high frequency applications. The team succeeded in growing large single crystal MoS_2 domains on device quality substrates using chemical vapor deposition techniques and fabricate field effect transistors for high frequency applications. The team fabricated crystals with edge length of >120 µm and fabricated RF FETs with fT = 20 GHz and cascode circuits with fmax = 2.9 GHz. Transistors with Ion/Ioff = 108 and saturation velocity of 1.88 x 106 cm/s were demonstrated. These technological advances transitioned to ARL-SEDD for further evaluation and development.

B. Novel Optical Microprobes for Ultra-Precise Intraocular Laser Surgery

Investigator: Professor Vasily Astratov, University of North Carolina - Charlotte, Single Investigator Award

Results of this research project, focused on microsphere-based optical imaging, transitioned to Wilmer Eye Institute for the development of scapels for retinal surgery, with the support of a grant from the National Eye Institue. Detachable scalpel tips that utilize a 5 microsphere (300um spheres) focusing element have been identified that provide for an extremely compact focal spot (50um) which are unperturbed by the surrounding tissue. This leads to a self-limiting penetration depth (10 um) and minimal thermal damage (30um) crater when used in conjunction with single Er:YAG laser pulses of 0.2 mJ and 75 ps duration. These values fall well below the values afforded by current intraocular fiber delivery systems. The collaborative research on application of novel optical scalpels in retinal surgery began with Dr. Howard Ying, an assistant professor of ophthalmology in the Wilmer Eye Institute and Applied Physics Laboratory at Johns Hopkins University. A similar collaborative effort also began with Dr. Andrew Antoszyk, a vitreoretinal surgeon at Charlotte Eye Ear Nose and Throat Associates.

C. Damage Precursor Detection and Mitigation

Investigator: Professor Aditi Chattopadhyay, Arizona State University, Single Investigator Award
Recipient: ARL-VTD

The objective of this research is to advance understanding of mechanochemistry by designing and demonstrating polymeric materials that can sense damage. A mechanophore-embedded thermoset polymer matrix (resin and cross-linker) was synthesized by embedding mechanophore units into networked epoxy to allow for damage detection by fluorescent emission. Both the cross-linker and the resin were modified by the addition of mechanophore units that, with UV curing, formed a network polymer crosslinked solely by stress-sensing/self-healing units, and a three-dimensional crosslinked polymer was formed due to the four reactive units on the cross-linker and the two reactive units on the resin. In FY17, these results transitioned to a newly-initiated collaborative effort between ARL-VTD in-house researchers with the goal of incorporating mechanophores into aerospace-grade structural composites. If successful, this joint effort will establish a new capability in damage precursor detection and mitigation for Army systems.

D. Combined Experimental and Computational Study of a Nanocrystalline Cu-Ta Alloy
Investigator: Professor Yuri Mishin, George Mason University, Single Investigator Award
Recipient: ARL-WMRD

The objective of this research is to study the stability of nanostructured alloys by performing a computational analysis of the relevant thermodynamic and kinetic factors using angular dependent interatomic potential calculations. This research transitioned to a collaboration with Drs. Darling and Hornbuckle at ARL-WMRD and Professor Kiran Solanki at Arizona State that combines the computational methods developed in this grant with an experimental study using a transmission electron microscope. In FY17, this collaboration resulted in a co-authored publication that reported that the high temperature stability of a nanocrystalline Cu-Ta alloy was due to kinetic influences arising from the formation of Ta nanoclusters near the grain boundaries, rather than thermodynamic forces. It was also found that the strain that resulted from the lattice misfit between the Ta clusters and the Cu matrix has a strong influence on the mechanical properties of the material, allowing it to retain a high strength even at elevated temperatures. It is anticipated that this collaboration will enable future advances in ARL's nanocrystalline alloy research, by providing a tool for identifying the relevant factors for attaining stability and improved mechanical properties in nanostructured alloys.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Quantum Devices Based on 2D Atomic Crystals and Their Heterostructures
Professor Novoselov Konstantin, University of Manchester, Single Investigator Award

The objectives of this project are to study the optical properties of novel two dimensional (2D) materials and to determine new methods for the fabrication of quantum emitters in 2D materials. Recently ferromagnetic 2D materials attracted a lot of attention. Such materials are interesting because there is a possibility to control spin properties of charge carriers in van der Waals heterostructures using such 2D ferro-magnets. It is anticipated that the optical properties of 2D magnetic materials such as $CrBr_3$, CrI_3 will be measured for the first time. The stability of the crystals and the photoluminescence spectra on the encapsulated and non-encapsulated materials will be investigated. Temperature dependence of photoluminescence of $CrBr_3$, CrI_3 from 6 K-room temperature will be measured. Bias dependence of electroluminescence of these materials are also anticipated.

B. Nanometer Scale Magnetic Resonance Imaging of Electron and Nuclear Spins
Professor Rafi Budakian, University of Waterloo, Single Investigator Award

Nanoscale magnetic resonance imaging (MRI) is on the verge of being realized. This technique will afford atomic-scale structural data with chemical specificity. This capability has never been demonstrated on the atomic scale, mainly because it requires very large time dependent magnetic field gradients in combination with long spin-coherence times. Both of these requirements have now been satisfied, and it is anticipated that the long-standing dream of high resolution MRI and spectroscopy at the nanoscale (below 2 nm) will be realized in FY18. This technique is expected to prove especially useful for determining protein structures.

C. In-situ Characterization of the Flash Sintering Process via Raman Spectroscopy
Professor Daniel Shoemaker, University of Illinois Champaign - Urbana, Single Investigator Award

The objective of this research is to characterize the process of flash sintering in-situ. The precise mechanisms of flash sintering, the rapid consolidation of a ceramic material subjected to an electric field and high temperature, remain controversial. The research team has built a custom flash sintering furnace designed to enable an UV Raman Spectrometer to capture spectra during the flash sintering process (see FIGURE 7). During FY18, it is expected that the first flash experiments will be performed and UV Raman Spectroscopy will be employed to measure the formation and kinetics of atomistic defects. As many of the proposed explanations for flash sintering conjecture that the electric field creates or influences atomistic defects in a manner that promotes rapid consolidation, this work could generate experimental data that resolves some of the ongoing debates in the field. Understanding the flash process should facilitate further development of this new processing method, enabling a means rapidly consolidating highly refractory ceramic materials.

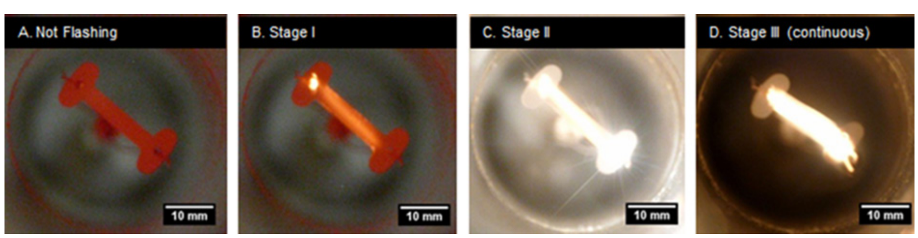

FIGURE 7

Stages of the flash sintering process for yttria stabilized zirconia. At a critical temperature, the current starts building in Stage 1, leading to an optical flash that can be analyzed with Raman Spectroscopy in Stage 2. At Stage III the flash is continuous and can be maintained for a prolonged period.

D. Degenerate Torque Materials for Cloaking in Elastic Media
Professor Guoliang Huang, University of Missouri - Columbia, Single Investigator Award

The objective of this research effort is to investigate elastic cloaking phenomena within a new class of materials that exhibit a unique set of collapse mechanisms and torque-induced non-symmetric stress states (i.e., Degenerate Torque Materials; DTMs). The work will seek to establish a theoretical framework for the modelling of DTMs and the inverse problem of design of specific DTMs targeting particular macroscopic constitutive parameters (typical of those required by elastic cloaks). The research will accordingly explore paths towards the design and fabrication, as well as dynamic modeling and homogenization, of specific degenerate mechanical trusses and lattices admitting collapse mechanisms and exhibiting aptitude for the support of body torque densities and non-symmetric stresses, such as chiral isostatic lattices. It is anticipated that in FY18 these researchers will develop and characterize a novel class of DTMs that possess a set of reliable collapse mechanisms and readily admit torque-induced non-symmetric stress states.

VI. DIVISION AND DIRECTORATE STAFF

A. Division Scientists

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Division Chief
Program Manager, Physical Properties of Materials

Dr. David M. Stepp
Program Manager (Acting), Mechanical Properties of Materials

Dr. John Prater
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CHAPTER 8: MATHEMATICAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2017* is to provide an annual historical record summarizing the programs and basic research supported by ARO in FY17. ARO's mission is to support creative basic research resulting in new science that enables new materials, devices, processes, and capabilities for the current and future Soldier. This chapter provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions enabled by the ARO Mathematical Sciences Division in FY17.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Mathematical Sciences Division supports research to develop a foundational framework for the understanding and modeling of complex nonlinear systems, for stochastic networks and systems, for mechanistic models of adaptive biological systems and networks, and for a variety of partial differential equation (PDE) based phenomena in various media. These research areas focus on discovering nonlinear structures and metrics for modeling and studying complex systems, creating theory for the control of stochastic systems, spatial-temporal statistical inference, data classification and regression analysis, predicting and controlling biology through new hierarchical and adaptive models, enabling new capabilities through new bio-inspired techniques, creating new high-fidelity computational principles for sharp-interface flows, coefficient inverse problems, reduced-order methods, and computational linguistic models. This research will ensure the U.S. is on the research frontier in mathematical sciences, and will enable new advances in disciplines that depend on mathematics.

2. Potential Applications. Research managed by the Mathematical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. Long term basic research discoveries regarding the modeling of complex systems may enable full (*i.e.*, not only physical) situational awareness through modeling of urban terrain and small-group social phenomena. Outcomes of basic research in probability and statistics may provide enhanced levels of information assurance, improved awareness of and defense against terrorist threats, next generation communication networks, and improved weapon design, testing, and evaluation. New discoveries in biomathematics may lead to protection against future biological and chemical warfare agents, improve wound-healing, lead to self-healing communication networks, enhance cognitive capabilities for the Soldier, and contain or prevent infectious disease. Advances from basic research in the area of numerical analysis may enable faster/better analysis, design, prediction, real-time decision making, and failure autopsy.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives and to maximize the impact of potential discoveries for the Army and the nation, the Mathematical Sciences Division frequently coordinates, leverages, and transitions research within its Program Areas with other ARL Campaign scientists and engineers, such as in Assessment and Analysis (e.g., novel mathematically rigorous statistical reliability and survivability methods), Computational Sciences (e.g., stochastic quantum differential equations for quantum computing), Human Sciences (e.g., structured methods for machine translation of low resource languages), Information Sciences (e.g., mathematical formulation of the dynamics of topologically-changing communication systems which serve as basis of system control methods), Materials Research (e.g., mathematics of incommensurability for multiscale modeling of 2-D materials), Sciences for Maneuver (e.g., isogeometric analysis for turbine design), and Sciences for Lethality and Protection (e.g., design of experimental techniques for meager data sets). The Division's research portfolio also supports the ARL ERAs of (i) Intelligent Teams, (ii) Impact of Operating in a Contested Environment, and (iii) Implementation.

The Division also coordinates and leverages research with other DoD agencies such as the Office of Naval Research (ONR) and the Air Force Office of Scientific Research (AFOSR). In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the Network Sciences Division pursue common interests in cognitive modeling, bio-network modeling and design, and new concepts in computational optimization. The Mathematical Sciences Division also coordinates its research portfolio with the Computing Sciences Division to promote investigations of new architectures and algorithms for the future of heterogeneous computing and to pursue related interests in image recognition and information fusion. Research also complements initiatives in the Life Sciences Division to model and understand the relationship between microbial growth conditions and composition, leading to advances in microbial forensics. The creation of new computational methods and models to better understand molecular structures and chemical reactions are an area of collaboration between the Chemical Sciences and Mathematical Sciences Divisions. The Mathematical Sciences Division also coordinates its research portfolio with the Physics Division to pursue fundamental research in the stochastic PDEs of quantum control. The Division interfaces with Program Areas in the Mechanical Sciences Division to explore the mechanics of fluids in flight and to better understand combustion. These interactions promote synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

The Mathematical Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY17, the Division managed research within these four Program Areas: (i) Modeling of Complex Systems, (ii) Probability and Statistics, (iii) Biomathematics, and (iv) Computational Mathematics. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Modeling of Complex Systems. The goal of this Program Area is to develop quantitative models of complex, human-based or hybrid physics and human-based phenomena of interest to the Army by identifying unknown basic analytical principles and by using human goal-based metrics. Complete and consistent mathematical analytical frameworks for the modeling effort are the preferred context for the research, but research that does not take place in such frameworks is considered if the phenomena are so complex that such frameworks are not feasible. The identification of accurate metrics is part of the mathematical framework and is of great interest, as traditional metrics often do not measure the characteristics in which observers in general, and the Army in particular, are interested. For many complex phenomena, new metrics need to be developed at the same time as new models. This Program Area is divided into two research thrusts: (i) Geometric and Topological Modeling and (ii) Small-group Social and Sociolinguistic Modeling. In FY13, the Modeling of Complex Systems Program included legacy efforts in information fusion. New efforts in information fusion will be part of the Information Processing and Fusion Program in the ARO Computing Sciences Division.

This Program Area develops mathematical analysis for fully 3D (rather than 2.5D) geometric and topological modeling of large urban regions up to 100 km x 100 km, which is important for situational awareness, mission planning and training. It develops the quantitative, analytical models of small social groups and of sociolinguistic phenomena which are required for operations, training, simulation (computer generated forces) and mission planning.

2. Probability and Statistics. The goal of this Program Area is to create innovative theory and techniques in stochastic/statistical analysis and control. Basic research in probability and statistics will provide the scientific foundation for revolutionary capabilities in counter-terrorism, weapon systems development, and network-centric warfare. This Program Area is divided into two Thrust areas: (i) Stochastic Analysis and Control, and (ii) Statistical Analysis and Methods.

The goal of the Stochastic Analysis and Control Thrust is to create the theoretical foundation for modeling, analysis, and control of stochastic networks, stochastic infinite dimensional systems, and open quantum systems. Many Army research and development programs are directed toward modeling, analysis, and control of stochastic dynamical systems. Such problems generate a need for research in classical and quantum stochastic processes, random fields, and/or classical and quantum stochastic differential equations in finite or infinite dimensions. These systems often have non-Markovian behavior with memory for which the existing stochastic analytic and control techniques are not applicable. The research topics in this Thrust include, but are not limited to, the following: (i) analysis and control of stochastic delay and partial differential equations; (ii) complex and multi-scale networks; (iii) spatial-temporal event pattern analysis; (iv) quantum stochastics and quantum control; (v) stochastic pursuit-evasion differential games with multi-players; and (vi) other areas that require stochastic analytical tools.

The objective of the Statistical Analysis and Methods Thrust is to create innovative statistical theory and methods for network data analysis, spatial-temporal statistical inference, system reliability, and classification and regression analysis. The research in this Thrust supports the Army's need for real-time decision making under uncertainty and for the design, testing and evaluation of systems in development. The following research topics are of interest to the Army and are important for providing solutions to Army problems: (i) Analysis of very large or very small data sets, (ii) reliability and survivability, (iii) data, text, and image mining, (iv) statistical learning, (v) data streams, and (vi) Bayesian and non-parametric statistics, (vii) statistics of information geometry, and (viii) multivariate heavy tailed statistics.

Potential long-term applications for research carried out within this Program Area include optimized design and operation of robust and scalable next-generation mobile communication networks for future network-centric operations made possible through advances in stochastic network theory and techniques. Also, advances in stochastic fluid turbulence and stochastic control of aerodynamics can improve the maneuvering of helicopters in adverse conditions and enable optimal design of supersonic projectiles. In addition, new results in density estimation of social interactions/networks will help detect adversarial behaviors and advances in spatial-temporal event pattern recognition and will enable mathematical modeling and analysis of human hidden intention and will provide innovative approaches for counter-terrorism and information assurance. Finally, new discoveries in signature theory will significantly improve reliability of Army/DoD systems and experimental design theory, and will lead to accurate prediction and fast computation for complex weapons.

3. Biomathematics. The goal of this Program Area is to identify and mathematize the fundamental principles of biological structure, function, and development across biological systems and scales. The studies in this program may enable revolutionary advances in Soldier health, performance, and materiel, either directly or through bio-inspired methods. This Program Area is divided into three main research Thrusts: (i) Multiscale Modeling/Inverse Problems, (ii) Fundamental Laws of Biology, and (iii) Modeling Intermediate Timescales. Within these thrusts, basic, high-risk, high pay-off research efforts are identified and supported to achieve the program's long-term goals. Research in the Multiscale Modeling/Inverse Problems Thrust involves creating mechanistic mathematical models of biological systems at different temporal and/or spatial scales and synchronizing their connections from one level of organization to another, with the goal of achieving a deeper understanding of biological systems and eventually connecting top-down and bottom-up approaches. Research in the Fundamental Laws of Biology Thrust is high-risk research in biomathematics at its most fundamental level, seeking to find and formulate in a mathematical way the basic, general principles underlying the field of biology, a feat that has been performed for other fields, such as physics, but is in its infancy with respect to biology. Efforts in the Modeling at Intermediate Timescales Thrust attempt to develop new methods of modeling of biological systems, as well as their control, at intermediate timescales.

While these research efforts focus on high-risk, high pay-off concepts, potential long-term applications for the Army include new and better treatments for biowarfare agent exposure, improved military policies on troop movements in the presence of infectious disease, optimized movements of groups of unmanned autonomous vehicles and communications systems, and improved understanding of cognition, pattern recognition, and artificial intelligence efforts. Research in this Program Area could also lead to improved medical diagnoses, treatments for disease, limb regeneration, microbial forensics, detection of terrorist cells, and self-healing networks. Finally, efforts within this program may result in a revolutionized understanding of biology in general, which will at the very least allow future modeling efforts to be much more efficient and also undoubtedly have far-reaching effects for the Army in ways yet to be imagined.

4. Computational Mathematics. The goal of this Program Area is to develop a new mathematical understanding to ultimately enable faster and higher fidelity computational methods, and new methods that will enable modeling of future problems. The research conducted within this program will enable the algorithmic analysis of current and future classes of problems by identifying previously unknown basic computational principles, structures, and metrics, giving the Army improved capabilities and capabilities not yet imagined in areas such as high fidelity modeling, real-time decision and control, communications, and intelligence. This Program Area is divided into three research Thrusts: (i) Multiscale Methods, (ii) PDE-Based Methods, and (iii) Computational Linguistics. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goals. The goal of research in the Multiscale Methods Thrust is to achieve higher fidelity and more efficient modeling of multiscale phenomena in a variety of media, and to create general methods that make multiscale modeling accessible to general users. Efforts in the PDE-Based Methods Thrust focus on developing the mathematics required for higher fidelity and more efficient modeling of sharp-interface phenomena in a variety of media, to discover new methods for coefficient inverse problems that converge globally, and to create reduced order methods that will achieve sufficiently-accurate yet much more efficient PDE solutions. Efforts in the Computational Linguistics Thrust focus on creating a new understanding of natural language communication and translation through new concepts in structured modeling.

While these research efforts focus on high-risk, high payoff concepts, potential long-term applications for the Army include force protection concrete and improved armor, more stable but efficient designer munitions, high density, rapid electronics at low power, and nondestructive testing of materials. Program efforts could also lead to more capable and robust aerial delivery systems, more efficient rotor designs, systems to locate explosive materials, more efficient combustion designs, and real-time models for decision-making. Finally, efforts within this program may lead to natural language interactions between bots and humans in cooperative teams, new capabilities for on-the-ground translation between deployed U.S. forces and locals, especially in low-resource language regions, new and improved capabilities for automated translation, automatic summarization, and textual analysis within the strategic intelligence communities.

C. Research Investment

The total funds managed by the ARO Mathematical Sciences Division for FY17 were \$20.5 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY17 ARO Core (BH57) program funding allotment for this Division was \$7.1 million and \$1.5 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided \$8.1 million to projects managed by the Division. The Division also managed \$2.2 million of Defense Advanced Research Projects Agency (DARPA) programs and \$0.2 million provided by other Federal agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided \$0.7 million for contracts. In addition, \$2.1 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MSI) Programs, including funding for DoD-funded Partnership in Research Transition (PIRT), DoD-funded Research and Educational Program (REP) projects, and \$1.4 million of the Division's ARO Core (BH57) funds, with the latter included in the BH57 subtotal above.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY17 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY17 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY17, the Division awarded thirty new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Erol Akcay, University of Pennsylvania; *A General Theory of Social Structure Integrating Demography and Decisions on Social Networks*
- Professor Ravi Allada, Northwestern University; *Multisensory Integration by Circadian Clocks*
- Professor John Benedetto, University of Maryland; *New Data Dependent Mathematical Methods to Achieve Super-Resolution*
- Professor Shankar Bhamidi, University of North Carolina - Chapel Hill; *Probabilistic models for network growth, change point detection and emergence of self-organization through reinforcement*
- Professor Dana Boatman, Johns Hopkins University; *A New Cross-Frequency Granger Causality Method for Investigating Cortical Dynamics*
- Professor Wei Cai, Southern Methodist University; *Efficient Numerical Methods for Stochastic Modeling of Optical Absorption in Solar Cells*
- Professor Richard Charnigo, University of Kentucky; *Almost-Smooth Nonparametric Regression and Pattern Recognition*
- Professor Kaushik Dayal, Carnegie Mellon University; *A Multiscale Atomistic Method for Long-Range Electrical Interactions Accounting for Finite-Temperature Thermal Fluctuations*
- Mr. Charles Fisher, Applied Research Associates; *Multi-Fidelity TBI*
- Professor Parag Katira, San Diego State University; *Predicting Tissue Dynamics Based on Stochastic Variations in Cell Stiffness and Spatial Clustering Within the Tissue Environment*
- Professor Nancy Kopell, Boston University; *Role of REM Sleep in Emotional Memory Consolidation with Implications for Post-Traumatic Stress Disorder*
- Professor Leonid Koralov, University of Maryland - College Park; *Multi-Scale Problems in Stochastic*
- Professor Vasileios Maroulas, University of Tennessee – Knoxville; *Construction of Distributions on Complex Topological Spaces of Signals and Their Application to Machine Learning and State Estimation*

- Professor Alex Mogilner, New York University; *Mathematics of Collective Cell Migration in Electric Field*
- Professor Daniel Onofrei, University of Houston; *Field Control through Submanifold Active Manipulation in CED*
- Professor Guodong Pang, Pennsylvania State University; *Ergodic Control of Large-Scale Stochastic Networks*
- Professor James Peterson, Clemson University; *Complex Models on Graph Based Topological Spaces*
- Professor Josh Plotkin, University of Pennsylvania; *Inferring the Role of Epistasis in Molecular Evolution*
- Professor Xiaoping Qian, University of Wisconsin - Madison; *Compatible Parameterizations based Isogeometric Analysis of Fluid-Structure Interaction with Applications in Blast Mitigation*
- Professor Shohei Shimizu, Shiga University; *Causal Feature Learning*
- Professor Suzanne Sindi, University of California – Merced; *Incorporating Uncertainty to Improve Accuracy in Mathematical Modeling of Coagulation*
- Professor Huan Sun, Ohio State University; *Advancing Human and Machine Question Answering via Human-Machine Collaboration*
- Professor Daisuke Takagi, University of Hawaii - Honolulu; *Transient Behavior of Organisms Responding to Sudden Cues*
- Professor Jonathan Taylor, Stanford University; *Interactive Data Analysis With Statistical Guarantees*
- Professor Tayfun Tezduyar, Rice University; *Multiscale Space-Time Methods for Fluid-Structure Interaction Analysis with Topology Change, Slip Interfaces and Thermal Effects*
- Professor Denis Tsygankov, Georgia Institute of Technology; *An Integrative Methodology for the Multi-Scale Study of Collective Behavior Emerging in a Heterogeneous Cell Population*
- Professor John Wen, Rensselaer Polytechnic Institute; *A Quantitative Approach to the Biochronicity of Circadian Rhythm, Sleep, and Neurobehavioral Performance*
- Professor Chien-Fu Wu, Georgia Institute of Technology; *Sequential Designs For Sensitivity Testing And Computer Experiments*
- Professor Nail Yamaleev, Old Dominion University; *Physics-Based Spectral Collocation Methods for Large Eddy Simulation on Adaptive Grids*
- Professor Bin Yu, University of California - Berkeley; *Estimation and Model Selection in Heterogeneous High-dimensional Settings with Random Forests*

2. Short Term Innovative Research (STIR) Program. In FY17, the Division awarded six new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Fred Adler, University of Utah; *How Complex Systems Code with Noise: Balancing Centralized and Decentralized Control*
- Professor Tryphon Georgiou, University of California - Irvine; *Non-equilibrium Statistical Mechanics and Curvature*
- Professor Saralees Nadarajah, University of Manchester; *Bias reduction in population size estimation of big data*
- Professor Francisco Samaniego, University of California - Davis; *Research on Reliability and Comparative Inference*
- Professor Thomas Strohmer, University of California - Davis; *Toward an Algorithm for Fast Matrix Multiplication*
- Professor John Terilla, CUNY - Queens College; *Critical Language Modelling with Trace-Density Representations*

3. Young Investigator Program (YIP). In FY17, the Division awarded two new YIP projects to drive fundamental research in an area relevant to the current and future Army. The following PIs and corresponding organizations were a recipient of the new-start YIP award.

- Professor Justin Solomon, Massachusetts Institute of Technology, *Smooth Modeling of Flows on Graphs*
- Professor Yizao Wang, University of Cincinnati; *From Random Partitions To Self-Similar Processes*

4. Conferences, Workshops, and Symposia Support Program. The Division provided funds in support of a range of scientific conferences, workshops, and symposia that were held in FY17. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences, with the goal of supporting scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army, and to define the research needs, thrusts, opportunities, and innovation crucial to the future Army. Proposals requesting funding support, typically for less than $10K, were received and evaluated in line with the publicly available ARO BAA. In FY17, ten proposals were selected for funding by the Division in FY17 to support conferences, workshops, or symposia.

5. Special Programs. In FY17, the Division also awarded five new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school and undergraduate students. These efforts were funded through the ARO Core Program and Youth Sciences Programs, for research to be performed at academic laboratories currently supported through active SI awards (refer to CHAPTER 2, Section IX).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Mathematical Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Optimal Control of Quantum Open Systems. This MURI began in FY11 and was awarded to a team led by Professor Daniel Lidar of the University of Southern California. The goal of this MURI is to show a high degree of fundamental commonality between quantum control procedures spanning all application domains.

This research is pursuing the development of a new mathematical theory unifying quantum probability and quantum physics, and this research is developing new ideas in quantum control that are presently in their infancy. Of particular importance is perhaps the most pressing quantum control frontier: real-time coherent feedback control of non-Markovian open systems. To address this goal, the team is studying unifying features of controlled quantum phenomena. The means for achieving quantum control is generally categorized as either open-loop control, adaptive open-loop control, real-time feedback control, or coherent real-time feedback control. Despite the operational distinctions between these control categories, the researchers aim to show that there is a strong relationship between all of these approaches to control, using algebraic and topological techniques. This linkage is expected to be significant for seamlessly melding these tools together in the laboratory to draw out the best features of each method for meeting new control challenges and overcoming inevitable laboratory constraints, such as the context of proposed meso-scale laser and atomic Rb experiments.

2. Multivariate Heavy Tail Phenomena: Modeling and Diagnostics. This MURI began in FY12 and was awarded to a team led by Professor Sidney Resnick of Cornell University. The project aims to develop reliable diagnostic, inferential, and model validation tools for heavy tailed multivariate data; to generate new classes of multivariate heavy tailed models that highlight the implications of dependence and tail weight; and to apply these statistical and mathematical developments to the key application areas of network design and control, social network analysis, signal processing, network security, anomaly detection, and risk analysis.

More specifically, the researchers are investigating and developing statistical, mathematical, and software tools that will provide (i) flexible and practical representations of multidimensional heavy tail distributions that permit reliable statistical analysis and inference, allow model discovery, selection and confirmation, quantify dependence, and overcome the curse of dimensionality, (ii) heavy tailed mathematical models that can be calibrated which clearly exhibit the influence of dependence and tail weight and which are appropriate to the applied context, and (iii) exploitation of the new tools of multivariate heavy tail analysis to enable the study of social networks, packet switched networks, network design and control, and robust signal processing.

3. Associating Growth Conditions with Cellular Composition in Gram-negative Bacteria. This MURI began in FY12 and was awarded to a team led by Professor Claus Wilke of the University of Texas - Austin. The goal of this research is to develop methods to identify statistical association in multiple-input-multiple-output (MIMO) data using microbial growth and composition data.

To trace a microbe-causing disease to its source or to predict a microbe's phenotype in a given environment, it is necessary to be able to associate the conditions under which bacteria have grown with the resulting composition of the bacterial cell. However, the input and output data complexity – multiple, heterogeneous, and correlated measurements – poses an interpretational challenge, and novel methods for analyzing, integrating, and interpreting these complex MIMO data are sorely needed. The research team is thus comprised of experts in statistics, computational biology, computer science, microbiology, and biochemistry, with the goal of producing the following outcomes: (i) development of novel linear and nonlinear mathematical methods to associate bacterial cellular composition with growth conditions, (ii) identification of the types and ranges of growth conditions that lead to distinguishable cellular composition, (iii) identification of key compositional markers that are diagnostic of specific bacterial growth conditions, and (iv) assessment of model uncertainty, robustness, and computational cost. The MURI has developed capabilities in several novel areas of data analysis and statistics such as the analysis of MIMO data, the integration of side information into regression models, and inverse optimization approaches. In addition, the types of approaches developed in this project will advance DoD capabilities in bacterial forensics and enable natural outbreaks to be distinguished from intentional attacks.

4. Understanding the Skin Microbiome. This MURI began in FY14 and was awarded to a team led by Professor David Karig of the Applied Physics Lab at the Johns Hopkins University. The goal of this research is to develop a fundamental understanding of the forces shaping skin microbial communities across a range of spatial scales and to show how this understanding can be used to identify disease risk, predict disease outcomes and develop tools for disease prevention.

Human skin harbors diverse bacterial communities that vary considerably in structure between individuals and within individuals over time. The extent of this variability and its implications are not fully understood, nor is it known whether it is possible to predict what types of bacteria one is likely to find on the skin of a given individual. As a result, there are no effective tools to predict individuals more likely to acquire skin bacterial infections, then determine the efficacy of forensic analyses based on skin bacterial communities, nor to design novel strategies to limit the effective colonization of skin by pathogens. This project brings a variety of disciplines to bear on the problem: spatially explicit sampling, metagenomics, and bioinformatics will be used to characterize skin microbial communities at intermediate and large spatial scales. Molecular biology, analytical chemistry and synthetic biology will be used to probe smaller-scale processes that ultimately lead to larger-scale patterns. Ecological modeling will be used to integrate small-scale processes with large-scale patterns in order to arrive at a quantitative and predictive framework for interpreting the human skin microbiome. A series of models concentrating on four grand challenges will be built, tested and refined: (i) predicting microbiome composition based on environmental conditions, host state and microbe exposure patterns, (ii) identifying microbiome composition through volatile sensing, (iii) identifying disease risk through analysis of current state and anticipation of state changes, e.g., due to upcoming activities or events, and (iv) novel approaches for mitigating skin disease (e.g., optimal design of avoidance behavior, robustly engineered skin microbiomes). The results of this work will enable the manipulation of the skin microbiome in order to facilitate identification of allies, discourage bites of flying insects, predict skin disease, and as-yet-unimagined applications.

5. Strongly Linked Multiscale Models for Predicting Novel Functional Materials. This MURI began in FY14 and is awarded to a team led by Professor Mitch Luskin at University of Minnesota. The goal of this research is to investigate mathematical methods for strongly linking scales within the context of discovering novel functional materials.

Current research in multiscale modeling has moved little beyond weak dependence between continuum and atomistic models. In commonly-used weakly linked multiscale models, a macroscale exerts at most a homogeneous influence on a greatly separated finer scale and lacks constitutive properties, which are supplied by reaching down to the smaller scale to compute, average, and report back. Such weak multiscaling dilutes or eliminates nonlinearities and the resulting models misrepresent the observed macroscale behavior. Variabilities in microfunctional parameters not only generate uncertainty within a scale, but also propagate uncertainties between scales, both up and down, resulting in a potentially significant spread in macroscopic properties.

Removing degrees of freedom from a dense system during upscaling may result in loss of information that can only be accounted for by introducing suitable random and dissipative forces that render the final mathematical formulation stochastic. This project seeks to develop a mathematical foundation for a computational framework of several strongly linked scale models for functional materials, with attendant uncertainty quantification. This will be developed within the framework of designing and discovering novel perovskite materials, mismatched alloy semiconductor materials, and 2D nanomaterials with unprecedented functional properties.

6. Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications. This MURI began in FY16 and is awarded to a team led by Professor George Karniadakis at Brown University. The goal of this research is to develop a new rigorous theoretical and computational framework enabling end-to-end fractional modeling of physical problems governed by conservation laws in large-scale simulations.

Despite significant progress over the last 50 years in simulating complex multiphysics problems using classical (integer order) partial differential equations (PDEs), many physical problems remain that cannot be adequately modeled using this approach. Examples include anomalous transport, non-Markovian behavior, and long-range interactions. Even well-known phenomena such as self-similarity, singular behavior, and decorrelation effects are not easily represented within the confines of standard calculus. This project seeks to break this deadlock by developing a new class of mathematical and computational tools based on fractional calculus, advancing the field in specific areas of computational mechanics. The fractional order may be a function of space-time or even a distribution, opening up great opportunities for modeling and simulation of multiscale and multiphysics phenomena based on a unified representation. Hence, data-driven fractional differential operators will be constructed that fit data from a particular experiment, including the effect of uncertainties, in which the fractional PDEs (FPDEs) are determined directly from the data.

The work is addressing the fundamental issues associated with the construction of fractional operators for conservation laws and related applications. An integrated framework is being pursued that proceeds from the initial data-driven problem to ultimate engineering applications. This general methodology will allow the development of new fractional physical models, testing of existing models, and assessment of numerical methods in terms of accuracy and efficiency. The integrated framework is based on a dynamic integration of five areas: (i) mathematical analysis of FPDEs; (ii) numerical approximation of FPDEs; (iii) development of fast solvers; (iv) fractional order estimation and validation, from data; and (v), prototype application problems.

C. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY17, the Division managed two new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of two Phase I contracts that aim to bridge fundamental discoveries with potential applications. A list of STTR topics published in FY17 and a list of prior-year STTR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Historically Black Colleges and Universities / Minority Serving Institutions (HBCU/MSI) – New Starts

The HBCU/MSI program encompasses the (i) Partnership in Research Transition (PIRT) Program awards, (ii) DoD Research and Educational Program (REP) awards for HBCU/MSIs, and (iii) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY17, the Division managed one new REP award, in addition to active projects continuing from prior years. In addition, proposals from HBCU/MSIs are often among the projects selected for funding by the Division (refer to the list of HBCU/MSI new starts in *CHAPTER 2, Section IX*.

E. Defense University Research Instrumentation Program (DURIP)

No new starts were initiated in FY17.

F. Presidential Early Career Award for Scientists and Engineers (PECASE)-New Starts

No new starts were initiated in FY17.

G. DARPA Enabling Quantitative Uncertainty in Physical Systems (EQUiPS) Program

The DARPA EQUiPS Program builds on previous work in uncertainty quantification. Complex physical systems, devices, and processes important to the DoD are often poorly understood due to uncertainty in models, parameters, operating environments, and measurements. The goal of this program is to provide a rigorous mathematical framework and advanced tools for propagating and managing uncertainty in the modeling and design of complex physical and engineering systems. ARO co-manages the awards within this Program. Of particular interest are systems with multi-scale coupled physics and uncertain parameters in extremely high-dimensional spaces. Novel mathematical research is being developed for dealing with the underlying high dimensionality of the space of uncertain parameters, strong multi-physics coupling, and uncertainty in the models themselves. In addition, the lack of fundamental mathematical theory for decision making and design under uncertainty for these large-scale dynamic systems is being addressed though new methods for forward and inverse modeling to scale to high-dimensional multi-scale/multi-physics systems, a quantitative understanding of uncertainties and inadequacies in the physical models themselves, and a completely new paradigm for stochastic design and decision making for complex systems. This work helps further the work done in the Division's Computational Mathematics Program Area, Mathematics of Multiscale Modeling Thrust.

H. DARPA Models, Dynamics, and Learning (MoDyL) Program

Complex, nonlinear, multiscale dynamical systems are ubiquitous. Examples include weather, fluids, materials, biological systems, communication networks, and social systems. These systems often evolve to a critical state built up from a series of irreversible and unexpected events, which severely limits development and implementation of mathematical models to accurately predict formation and evolution of patterns in such systems. The Models, Dynamics and Learning (MoDyL) program aims to build rigorous data-driven models for non-equilibrium dynamics to address this challenge, leveraging existing data to enable robust prediction in complex systems. Collaboration among researchers from disciplines such as dynamical system theory, computational topology, statistics, spectral analysis, as well as domain experts in the various application problems is critical to address such a complex challenge. MoDyL will bring disparate researchers together to develop fundamental mathematics and computational algorithms for extracting models from dynamic data sets.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Mathematical Sciences Division.

A. Subspace Methods for Massive and Messy Data

Professor Laura Balzano, University of Michigan, Single Investigator Award

The goal of this research is to derive a robust sub-space tracking technique, which is an important modeling method for streaming data and machine learning in video and computer vision, power grid monitoring, environmental sensing, and communications (among other applications). Professor Balzano was part of the team that developed the current state-of-the-art algorithm in subspace identification and tracking, GROUSE – or *Grassmanian Rank-One Update Subspace Estimation*. GROUSE uses an incrementally updated, stochastic gradient approach to analyze the Grassmannian – or manifold of all subspaces – of the ambient data space. It is a step beyond previous subspace identification and tracking approaches not only in its speed and ease of implementation, but also in that it works even when the measurement vectors are highly incomplete. This is useful in situations where data being collected in large complex systems is often lost or corrupted in transmission, or in situations where only incomplete and continually updating data is necessary available, such as in recommender systems (e.g. customer recommendations in platforms like Amazon, Pandora, Netflix, etc.).

While more robust and significantly faster than other subspace tracking methods, the original GROUSE framework does struggle with *ill-conditioned* data, i.e., when there is a large dynamic range among the important signal components. One of the primary goals of this research has been to improve the performance on data with this characteristic.

In FY17, the final year of her ARO-sponsored project, Dr. Balzano extended the capabilities of the GROUSE framework to achieve high accuracy on a subspace estimate using half as many iterations as standard GROUSE for data with condition number up to 1000 (i.e. the largest data points are 1000x magnitude of the smallest). The research team defines “high accuracy” to be dependent on the noise level in each context, with a goal of getting to within 10 factors of the noise level as generated in a simulated data context, as is estimated in real data. This increase in computational speed and robustness with respect to conditioning was achieved by developing another extension of the algorithm which tracks a low-rank subspace model over time as an optimal basis is iteratively obtained. With this enhancement, the PI has already achieved advances in computational cost and speed in image and video processing, particularly in modeling the background of an image as a low-rank subspace and then separating the foreground activity, which holds for images that are blurred or distorted by camera motion.

Another method being investigated by the PI is subspace clustering, which models each cluster within the data as a low-dimensional subspace. This is a very common data analysis tool and is the model at the center of the PI’s current research in subspace methods applied to video and image identification and recognition. Current state-of-the-art subspace clustering algorithms are unsupervised and achieve best in class clustering error in recognition applications, but the error is still generally above ~10-15% on benchmark datasets. In FY17, the PI developed new algorithms and active learning methods to drive this error down, achieving an improvement in recognition accuracy over the current state-of-the-art with an error rate consistently below 10% when matching images to a fixed data base.

In yet another direction, the PI developed a new general algorithm for principal component analysis (PCA), another indispensable tool in studying large, incomplete data sets. The PI’s specific interest in this direction is in data that is received and/or processed sequentially, and for which limited storage or memory is available. The general objective of the method is to sequentially approximate a subspace S of the (generally very high dimensional) ambient data space with successive subspaces S_k in such a way as to ensure metric convergence of the subspaces S_k to the desired subspace S. This method is applicable in a large variety of contexts and applications (i.e. under mild requirements), with possibly highly incomplete or corrupted data, and by utilizing as little memory and storage as possible. Since the method compares the subspaces S and S_k using principal component analysis, the metric used to measure how far away the two subspaces are from each other – $d_G(S,S_k)$ –

is based upon measurements of the principal angles of the subspaces. The resulting algorithm is Subspace Navigation via Interpolation from Partial Entries, or SNIPE. SNIPE is an iterative, least change method, meaning that care is taken at each time step to balance the best approximation with the least change from the previous iterate, yielding optimal memory usage. The PI showed, both empirically and in formal mathematical proofs, that the estimation error, $d_G(S,S_k)$, decreases exponentially with respect with respect to the data sampling probability (see FIGURE 1). Furthermore, the sampling error decrease for SNIPE over a greater number of allowed iterations improves upon GROUSE and is significantly better than the more classical power method.

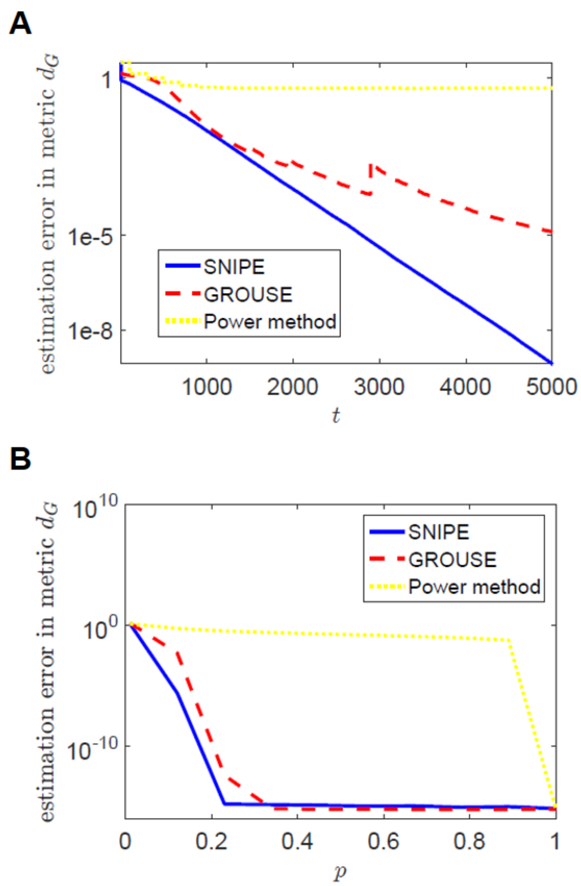

FIGURE 1

Subspace Navigation via Interpolation from Partial Entries (SNIPE) estimation error vs other methods. Estimation error vs. (**A**) time (in milliseconds) and (**B**) sampling probability p for SNIPE, GROUSE, and the modified power method.

B. Tomography of Social Networks of Asymmetric Adversaries

Professors Joe Blitzstein (Harvard University) and Patrick Wolfe (Cambridge University), MURI Award

The goal of this MURI, which ended in FY17, was to develop quantitative procedures to identify, characterize and display – on the basis of externally observed data generated from passive and/or active procedures – covert social networks of asymmetric adversaries, that is, terrorist/insurgent networks. This MURI began in FY10 and was awarded to a team originally led by Professor Patrick Wolfe, formerly of Harvard University and currently at Cambridge University. Changes in the team resulted in Professor Joe Blitzstein of Harvard coordinating the research over the final two years, with Professor Wolfe continuing to contribute. From the mathematical perspective, the question was thus posed: how, and under what conditions, can one detect the presence of structure in networks – structure that is not well explained by conventional background models?

In its first three years, the MURI team developed a framework for quantifying the fundamental limits of detectability for embedded insurgent sub-networks. This first rigorous "signal detection theory" for networks enables the computation of these performance limits within a coherent mathematical framework and the development of algorithms that approach them. This theory enables one to make trade-offs between algorithmic performance and computational requirements.

This was a significant mathematical advancement that essentially developed a new branch of mathematical network theory and statistical network analysis. In essence, the theoretical framework allows one to extract various separations of a larger, ambient network into background and foreground sub-networks by using deviations from a best fit model, and the resulting outliers in the model indicate sub-networks. More specifically, the model encodes "society + network" connections (e.g., adjacency matrix with elements $\neq 0$ if a connection exists) to fit a benign-background model to the encoded "society + network" model. A similar approach is then used to fit a notional "signal-plus-clutter" model to various partitions of the "society + network" model to make the network signal stand out from clutter. One of the results was the first ever decision-theoretic, mathematically rigorous theorem that allowed one to formally test for signal presence in sub-networks simply by observing if the sub-network structure is consistent with the fitted clutter model.

In FY17, the MURI team focused on actual detection more than general theory. They defined the various threads within community detection models. Within each thread, the team developed mathematical models that are based on sociological processes which tackle subgroup detection with respect to different sociological process (language, geolocation, densities of interaction, etc.). Each of these efforts demonstrated mathematical richness, with an apparent possibility to move closer to establishing error bounds on predictions. The effort based simulation structure on real terrorist networks with quality control evaluations.

C. Nonlinear and Probabilistic Analysis with Frames

Professor Radu Balan, University of Maryland - College Park, Single Investigator Award

One of the objectives of Professor Balan's research is the advancement of novel mathematical techniques to analyze nonlinear phenomena, with a particular interest in phase retrieval and quantum state tomography. Quantum Information Processing represents the foundation of such applications as quantum computing, quantum data encryption and distribution technology, as well as other types of data processing. The phase retrieval problem can be simply stated as recovery up to a global phase factor of an unknown vector from magnitudes of scalar products with a redundant set of vectors, and the quantum state tomography asks for recovery of a unit trace positive semi-definite symmetric form (from Hilbert-Schmidt scalar products with a set of self-adjoint operators). For reference, other examples of nonlinear phenomena include X-Ray crystallography, speech recognition, deep learning, and non-convex optimization, all of which use nonlinear processing of incomplete information.

In FY17, significant progress in these areas was achieved, especially the breakthrough on the quantum tomography problem that considers the estimation of a positive semidefinite matrix of unit trace, (which represents the quantum state), from a set of measurements, which are represented as linear projections of this matrix. Four important results on quantum keys distribution, quantum state detection and robust quantum state estimation are summarized here.

For quantum state detection, necessary and sufficient conditions for the frame quantum detection problem were derived for the finite dimensional and infinite dimensional cases, in both the real and complex Hilbert space. For the infinite dimensional case, it was discovered that frames which uniquely represent all the quantum states are not stable under perturbations and are rather rare. In other words, the set of quantum states are not dense in the class of all frames, which is a very surprising result.

Working towards constructing a quantum key distribution, Professor Balan's team created a method to compute companion equiangular tight frames by using the discrete Fourier matrix and a class of cleverly chosen generators. Specifically, for each prime number constructed, the companion equiangular tight frame is derived using a class of Legendre symbols applied on the Fourier equiangular tight frame. This class of companion equiangular tight frames are compatible with Zauner's conjecture, which asserts that in each dimension an equiangular tight frame can be constructed using a discrete Heisenberg group. While the full conjecture is still open, infinite families of equiangular tight frames generated by nonabelian discrete groups, including the finite Heisenberg group, were derived by applying Gelfand pairs as special cases of general Schurian association schemes. The previously described method gives theoretical evidence in favor of Zauner's conjecture.

Considering robust quantum detection, Professor Balan and his team derived techniques to analyze low-rank quantum states and to estimate low-rank quantum states in the presence of noisy measurements. The pure state case, when the quantum state has rank one, is addressed by the phase retrieval problem when the problem reduces to analysis on the projective space. The natural distance on projective space generalizes to the Bures/Hellinger distance on mixed states. Based on a recently proved inequality on the arithmetic mean of the geometric mean matrix, it was shown that finite dimensional quantum state estimation is always robust when the algebraic injectivity condition is satisfied. Furthermore, the projective space induced distance is Lipschitz was proven to be equivalent to the simpler Bures distance.

D. Warfighter Neuroendocrinology: Modeling Stress Response, PTSD, and TBI
Professor Maria D'Orsogna, California State University - Northridge, Single Investigator Award

The goal of this research is to develop and analyze a mathematical model that includes the relevant physiological features involved in stress response regulation. Stress-related disorders affect multiple biological functions from endocrine system regulation to brain circuitry connectivity. Identifying the mechanisms that lead to the development of such disorders has been an active area of research, with a particular emphasis placed on understanding the dynamics of post-traumatic stress disorders (PTSD). Although many advances have been made, how PTSD emerges and evolves is still unclear. Experimental studies have been challenged by incongruent diagnostic criteria and confounding treatment protocols. Although PTSD is often associated with low levels of cortisol, to date there is no reliable biological predictor or marker for PTSD and diagnoses are heavily reliant on self-reporting. Current treatments include psychotherapy and pharmacotherapy: it is not very clear how the two intervention methods inform each other and they are not always very successful. In part, these challenges are due to the lack of a comprehensive understanding of the biological processes and systems that are affected by PTSD and how they respond and interact with each other under stress.

In FY17 the researchers formulated a more complete and realistic model for the HPA axis where hitherto neglected processes were included (see FIGURE 2). Specifically, they distinguished the (slow) process of cortisol-mediated CRH biosynthesis from the (fast) process of CRH secretion. Their multi-time scale model was thoroughly analyzed using dynamical system and numerical methods and was able to reproduce known oscillatory behavior patterns. In addition, they uncovered the existence of two basins of attraction, one marked by "normal" cortisol levels, the other by hypocortisolism, which was considered to be the "diseased" state as is observed in PTSD patients. They found that external distress, such as due to traumatic events, can lead to transitions from the normal to the diseased state; this fact is important because it means that the emergence of hypocortisolism in PTSD patients can be due solely to psychological trauma and not necessarily because of physical injuries.

Given that external distress can cause normal-to-diseased transition the researchers also asked whether the reverse transition could be stimulated. Indeed, they found that by carefully tuning external stress, the reverse transition from diseased to normal state could be triggered. This result implies that exposure therapy, i.e. subjecting patients to stressful events in a clinical setting with the purpose of alleviating PTSD symptoms, may indeed help normalize HPA axis functionality. This analysis provides a causative rationale for improving treatments and guiding the design of new psychological protocols. Finally, they showed that timing and intensity of the external stress play a crucial role in determining how and if transitions occur.

The research team also performed parameter sweeps and found different behavioral regimes, which may be useful in determining the effects of physical trauma on the HPA axis functionality, where parameters are changed due to brain injuries, for instance. Bistability was found to emerge only under some parameter combinations that while defining a significant portion of parameter space are not exhaustive. This means that the subgroup of individuals that are represented by parameters that do not lead to bistability may be less susceptible to the onset of PTSD, compared to others.

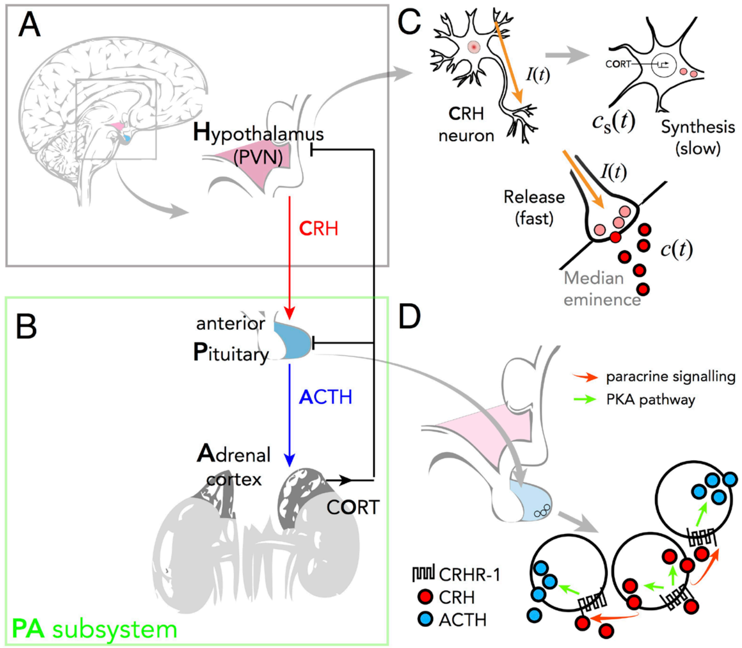

FIGURE 2

Schematic of the HPA axis. (A) Stress is processed in the central nervous system (CNS) and a signal is relayed to the paraventricular (PVN) in the hypothalamus to activate CRH secretion into the hypophyseal portal system. (B) CRH diffuses to the pituitary gland and activates ACTH secretion. ACTH travels down to the adrenal cortex to activate cortisol. (CORT) release. Cortisol inhibits both CRH and ACTH secretion to down-regulate its own production, forming a closed loop. (C) Negative feedback of cortisol suppresses CRH synthesis in the PVN, ultimately reducing the amount of stored CRH and its subsequent release. External inputs such as stressors and circadian inputs directly affect the release rate of CRH at the axonal terminal. (D) CRH released by the PVN stimulates the protein kinase A (PKA) pathway to activate release of CRH by the anterior pituitary, contributing to ACTH secretion in an auto/paracrine fashion.

Finally, the model was used to better understand the mechanisms underlying current clinical protocols used to probe patient stress response. Specifically, they addressed dexamethasone (DEX) and ACTH challenge tests, which probe the response of pituitary and adrenal gland responses, respectively. The model shows that adrenal hypo-sensitivity can give rise to the responses seen in ACTH challenge tests, and enhanced cortisol-mediated suppression of the pituitary in subjects with PTSD is not necessary to exhibit the responses observed in DEX stress tests. Finally, they proposed new two-stage DEX/external stressor protocols to better understand pituitary hormone suppression.

E. Finite Element Approximation of Nonlinear Systems Developing Shocks, Fronts and Interfaces

Professors Jean-Luc Guermond and Bojan Popov, Texas A&M University, Single Investigator Award

The objective of this research is to solve a hyperbolic system using continuous finite elements on non-uniform grids in any space dimension. To do this, the team has pursued the rigorous formalization of the notion of invariant domain for the approximation of hyperbolic systems using continuous finite elements. This approach generalizes the maximum principle concept to hyperbolic systems. This property is important in ensuring the positivity of the density and the internal energy and the minimum principle on the specific entropy in the compressible Euler equations and the Shallow water equations. This investigation pursues a general method of solving hyperbolic systems in any space dimension using forward Euler time steps and continuous finite elements on non-uniform grids. The properties of the method are based on the introduction of an artificial dissipation that is defined so that any convex invariant set containing the initial data is an invariant domain for the method. The invariant domain property is proven for any hyperbolic system provided the computation is done with sufficient resolution to resolve passage across a single domain element (i.e., the Courant–Friedrichs–Lewy condition holds). The solution is also shown to satisfy a discrete entropy inequality for every admissible entropy of the system. The method is formally first-order accurate in space and can be made high-order in time by using existing strong stability preserving algorithms. The project has been able to achieve provable positivity for second-order continuous finite elements for any hyperbolic system containing one or more scalar equations, such as for mass (see FIGURE 3).

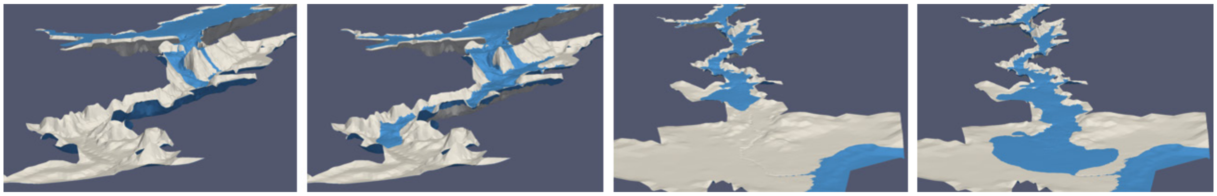

FIGURE 3

The dam break problem modeled as a hyperbolic system via continuous finite elements. The geometry modeled above is for the Malpasset dam in France which famously failed in 1959, modeled at four different times after dam break. New methods enable algorithms that do not require specialized effort or knowledge to enforce conservation laws in variously-discretized systems. This opens the way for exactly-conservative methods of general applicability, in a number of different computational frameworks or bases, suitable for use in general packages or by generalist users.

In FY17, several very significant advances were achieved. First, it establishes a general solution method for hyperbolic systems based on continuous finite elements; none was available prior to this investigation. It rigorously corrects the mistaken notion that one cannot approximate hyperbolic system with continuous finite elements because they are not "exactly conservative". This is achieved by identifying the ambiguities in the several current definition in the context of finite elements, and narrowing and sharpening the mathematical definition of conservation in this context. This project introduces a new first-order method that works for any hyperbolic system, with continuous finite elements, in any space dimension, on any non-uniform mesh. It is conservative in the sense that the total mass is always conserved if there is zero mass flux at the boundary. It introduces the most general result of this type, with the possible exception of the piecewise constant Discontinuous Galerkin method. The only limitation, that may yet be removed, is that the lumped mass matrix be non-negative. Most continuous finite elements satisfy this property. The key advance in the success of this method is the definition of the artificial viscosity, abandoning the traditional element-based weak form of the Laplacian operator and instead using a Graph Laplacian viscosity. This enables handling any mesh geometry without any constraint on the angles of the triangulation. This is a big conceptual leap forward that enables that will work without any tuning or special expertise from the user. This method is likely to assist any graduate student or engineer, with very little specialized education in hyperbolic equations, to program these methods by using any finite element toolbox.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Inferring Social and Psychological Meaning in Social Media (SURF)

Investigator: Mr. Tod Hagan, Securboration Inc., Small Business Innovation Research Award
Recipients: ARL Computational Sciences and Information Directorate (ARL-CISD), U.S. Army Special Operations Command (USASOC), NATO

The objective of this research has been to develop analytical tools that use structured and non-structured social media information to identify individual features of social media users by detecting significant topologies and motifs within online communities. Securboration, Inc. has developed and prototyped the *Social Understanding and Reasoning Framework* (SURF) to find and classify individuals through their social media networks. Demonstrations using SURF to analyze Twitter social networks achieved 85% or greater accuracy in classifying users into various categories, including ISIS sympathizers, hackers, and political influencers.

SURF finds and classifies social media users using only subnetwork motifs and learned repetitions of patterns of subnetwork usage. In short, it uses subnetwork geometry and topology, and nothing else. This is an innovation above the standard content-based social media analysis, and it allows operators to classify social media users in a way that is both language agnostic and content independent. For example, an ISIS sympathizer on Twitter or Facebook who uses fake photographs and a language different from his/her native language would not go undetected from SURF, since the false content would not alter the user's usage patterns and network interactions. SURF has been successfully tested on multiple language platforms, and it can consistently classify users into various categories (e.g. ISIS sympathizers, Arabic businessman, hackers, political influencers, etc.) at over 85% accuracy. Generally, any type of persona for which one can build a profile model may be used as a classification category.

During FY17, SURF was demonstrated to various agencies within the USASOC enterprise. Several agencies expressed desire to see SURF tested on real-time data and in operational situations, and a test was arranged that will continue into FY18. Finally, SURF was demonstrated to NATO partners at an Information Systems Technology Panel Research Specialist Meeting in September 2017. This demonstration led to the request by five of the participating nations for a multi-national series of experiments based around SURF, including variations in design, data feed, and scenario of application.

B. Prefrontal Brain Rhythms and Rule-Based Action

Investigator: Professor Nancy Kopell, Boston University, Single Investigator Award
Recipient: ARL Human Research and Engineering Directorate (ARL-HRED)

The objective of this research is to understand the impact of brain physiology on cortical oscillations and how these oscillations affect how the brain processes information. Neural oscillations are associated with all facets of cognition; nevertheless, the ways in which such brain dynamics support cognition is only beginning to be addressed. An understanding of how brain dynamics modulate and control learned rules that guide action can lead to a deeper understanding of the neural basis of higher cognitive activity. To address this question Professor Nancy Kopell built computational models constrained by *in vivo* and *in vitro* data, investigated the properties of these models by simulation, and applied the ideas to how the prefrontal cortex controls the execution of rule-based action.

This research has transitioned to collaborative studies between ARL researchers, Drs. David Boothe and Piotr Franaszczuk, and Professor Kopell. The researchers are focusing on the use of mathematical of modeling of the cerebral cortex to understand the relationship between brain features such as connectivity, physiology, and neuro-modulatory state and the generation of brain oscillations in the EEG relevant 1 to 100 Hz frequency range. Drs. Boothe and Franaszczuk are using techniques developed in the Kopell lab to enhance the empirical accuracy of

Army Research Laboratory's model of cerebral cortex. This research has the potential to improve human agent teaming through an improved understanding of soldier brain state, and could potentially be used to improve AI networks by allowing them to perform computation in a way that is similar to the human brain.

C. Binary and Hybrid Response Data in Sensitivity Testing: Sequential and Bayesian Optimal Designs
Investigator: Professor Chien-Fu Wu, Georgia Institute of Technology, Single Investigator Award
Recipient: ARDEC Picatinny Arsenal

An objective of this research is to develop mathematically rigorous uncertainty quantification (UQ) methods in the areas of (i) modeling and simulation (M&S) through specialized design of experimental techniques for computer simulations to develop a fast emulator to speed-up the computations, and (ii) the validation and verification (V&V) techniques to ensure that the M&S evaluations are reliable representations of how the technology would perform in the field. Professor Wu and co-PI, Professor Roshan, are working closely with the Statistics Group at ARDEC, collaborating on real-life problems faced by the engineers at ARDEC, which pose fundamental and challenging research problems in statistics.

Professors Wu an Roshan created the 3pod method, a sequential experimental design technique for sensitivity testing that is used for estimating the quantile of a distribution with minimum number of samples; the support points goodness-of-fit test, which determines a set of representative points for any given distribution by minimizing the energy distance; and the MaxPro technique, an experimental design that gives a set of points in a uniform hypercube to approximate the computer model with an approximate model (emulator) with few computer simulations (see FIGURE 4). The statistical methods and computer codes developed by the team have been transitioned to engineers at ARDEC, which are widely used in M&S in order to design, test, and optimize armament systems.

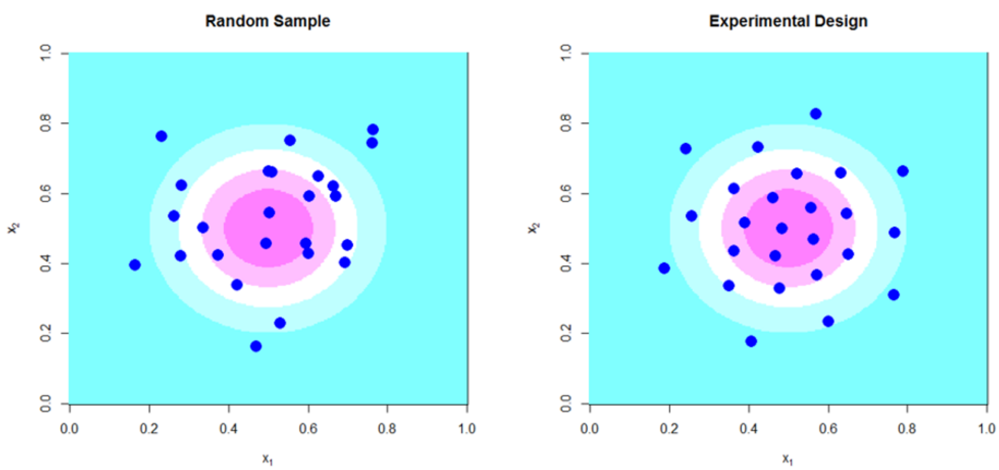

FIGURE 4

Comparison of the support points design method and Monte Carlo sampling for a bivariate normal distribution. The simulation displays that, when running a goodness-of-fit test, optimizing the energy distance finds the best sample of the distribution with a small amount of data points (Experimental Design), especially against Monte Carlo simulation (Random Sample), which will take a considerable amount of data points to span the distribution.

D. New Method to Compute the Fronts and Surfaces of Air Delivery, Combustion, and Aerodynamics
Investigator: Professor Xiaolin Li, State University of New York at Stony Brook, Single Investigator Award
Recipient: Natick Soldier Research and Development Center (NSRDEC)

The objective of this project is to investigate a very different method of efficiently computing the response of dynamic systems involving highly complex geometric interfaces immersed in the continuum medium, such as parachutes and parafoils. The usual method is through finite element methods, which require intricate discretizations, expert handling, and lengthy computations. These methods can be very powerful and very accurate, but very expensive in terms of time and resources, and generally require a nearly total restart when a different question is asked about changes such as unequal or breaking risers, sudden changes in loading, or others. A very different methodology has been investigated for the simulation of a parachute air deceleration system using the dual-stress spring mass model coupled with an incompressible fluid solver through the impulse method. The approach has been developed to simulate the parachute system based on the front tracking method. The data structure representing the fabric surface of the canopy has been designed to allow for the application of the computational library in the simulation of the dynamic motion driven by the gravitational force of the payload and the fluid pressure differential at the fluid-fabric interface; the discretized fabric surface is a homogeneously triangulated surface mesh. Angular stiffness has been added to the simple spring mass model in order for the model to conform to both the Young's modulus and Poisson ratio of the fabric. This duel-stress spring-mass model is coupled with the incompressible fluid solver with turbulence and porosity models. Realistic simulation tools include physically validated collision handling between different components of the system.

Proof of convergence has been carried out through numerical mesh refinement. While current methods require computing a very large number of quantities, the new method uses a far smaller number of simpler quantities that yield nearly the same result with far less computational effort and time. This research transitioned to NSRDEC, which then performed collaborative studies on the test use cases and jointly published three co-authored papers on the methods and results. This new method continues to be adapted for quickly analyzing new scenarios, such as the effect of unequal riser lengths on parachute integrity and accuracy, and parachute response when a riser breaks or is a twist occurs.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. From Random Partitions to Self-Similar Processes

Professor Yizao Wang, University of Cincinnati, Young Investigator Program Award

Stochastic models are commonly used to model various phenomena with significant amount of uncertainty, including for example the trajectory of a particle moving around in space, the fluctuations of internet traffic rates, or the landscape of random surface representing temperatures or rainfall amounts in environmental studies. A major research objective of Professor Wang is to derive techniques and methods to characterize behaviors of stochastic models. A ubiquitous phenomenon is when the stochastic model under investigation becomes large, or equivalently when investigating the aforementioned phenomena at a very large temporal or spatial scale, after appropriate scaling and normalization, different stochastic models may behave in very similar manners. The investigation of the limit stochastic processes then in turn provides methodologies and guidelines to the inference problems related to the phenomena.

The stationary sequences of interest arise from an aggregated nature, for instance, internet traffic through a certain router or the servers managing all the activities on tweeters. One of the main goals of the research is to create methods to determine limit theorems for the extremes of certain stationary sequences with long-range dependence. A unique feature of this class of models is the appearance of large values from different individuals in clusters and over a very long time span, and large values from different individuals may overlap in the limit. This is in drastic contrast to most other models, where large values do not cluster, or only cluster locally, and never overlap. It is anticipated in FY18 that Professor Wang will derive a complete picture of all large values at different ranks, including their clusters, locations, and overlaps. The anticipated results will be seen for the first time in the literature, and opens new directions in future research of stochastic processes with long-range dependence.

Another area investigated by Professor Wang is the aggregated random-field model; in probability theory and applications, a random field is typically used to model spatial phenomena with uncertainty. It is anticipated that in FY18 that the PI will establish that flexible Gaussian random fields that are self-similar and anisotropic. In other words, random fields that behave the same when looking at different scales, and the existence of subspaces where the model may exhibit drastically different behavior along different directions, respectively. It is also anticipated that Professor Wang will derive stochastic models for which a flexible family of anisotropic and self-similar Gaussian random fields arise in the limit. This result would justify the robustness and universality of the Gaussian random fields, which could then be considered as natural candidates in applications.

B. Construction of Distributions on Complex Topological Spaces of Signals and Their Applications to Machine Learning and State Estimation

Professor Vasileios Maroulas, University of Tennessee, Single Investigator Award

Robust analysis of complex systems, such as signal classification and clustering or state estimation in topological spaces of signals emitted by a sensor network, requires a colossal engagement of topology, geometry, statistics and machine learning. Signal classification investigates topological features of the point cloud data space, summarized by persistence diagrams (PDs) – the primary analytical tool in persistent homology and topological data analysis. Threat detection and assessment in a sensor network requires understanding the network topology by estimating hidden states of PDs, which compress necessary information about the network's connectivity. Previous studies have engaged statistical learning methods for PDs for addressing these problems by adopting artificial assumptions tailored to the application and the data under consideration. This ad hoc approach, along with the inability of current metrics related to PDs to handle the full range of statistical feature measures, shows that a general foundational strategy for analyzing PDs is desperately required for complex topological data analysis. An objective of this research proposes the construction of distributions of random PDs and an entirely new metric on the space of persistent diagrams that would be universally applicable to the space of PDs associated with any compact space. The PI will then establish a Bayesian framework for estimating conditional distributions of PDs associated with SN signals and will discover cutting-edge unsupervised and supervised learning methods.

A PD is a visualization tool that encapsulates the topological properties of the underlying dynamical space from which signals arise. Each point on a PD represents a topological feature through three inputs: a topological dimension (indicating a cluster or a high-dimensional hole) and the birth-death location of the feature. The PI will shed light on the investigation of PDs by constructing their probability distributions via finite set statistics, a strategy heretofore not tried in topological data analysis. Decomposing random PDs into a union of singleton sets, its distribution will depend on each single element's birth-death distribution. Overall, this novel approach will bridge the previous fractured body of recent work. For instance, statistical summaries of PDs like their mean and variance will be computed without relying on special properties of each problem's associated data space. Derivation of these summaries will lead to the establishment of innovative (un)supervised machine learning techniques by optimizing appropriate metrics from the distribution or mean of PDs under investigation. Furthermore, the newly proposed metric on the space of PDs – which is the primary tool used in classifying and differentiating signals from one another – would handle both general and finite state statistics equally well, which the "classical" Wasserstein metric does not.

It is anticipated that in FY18 the PI will provide both empirical and mathematically rigorous proofs that the proposed metric is viable and can accurately measure the distance between PDs. This metric will be the first of its kind in topological data analysis, in that it takes into account both the geometry of space of diagrams and the statistical analysis for which it is to be used. Bridging the gap between topological data analysis, statistical analysis of data, and machine learning has been a task of importance for several years, and most general approaches have examined the statistical side of the problem. This metric would be the first that spans that gap from the geometric side, measuring the distance with the statistics in mind, instead of trying to alter the statistical analysis to fit the imposed geometry. If the metric is shown to be viable, future work on this project will focus on the statistical analyses of various data sets and the correlation between statistical features and data geometry.

C. Predicting Tissue Dynamics Based on Stochastic Variations in Cell Stiffness and Spatial Clustering Within the Tissue Environment

Professor Parag Katira, San Diego State University, Single Investigator Award

The goal of this project is to understand how inter-cellular heterogeneity within cells forming biological tissues influences tissue level processes such as tissue regeneration, wound healing, aging and disease occurrence such as cancer. Using stochastic dynamical models of cell-cell interactions within simulated tissue environments, the migratory and proliferative behavior of individual cells, clustering rates of cells with similar phenotypes, and the influence of resulting changes in local and global heterogeneities in the cell population on overall tissue dynamics will be predicted.

Variations in the properties identifying individuals within a given population is the norm in biology. For example, every human being from a given population is different. This concept holds true at various hierarchical levels in biology all the way down to the individual cells that make up the tissues and organs of the body. Each cell is slightly different in its biochemical and biomechanical properties from the other cells that make up the tissue. Ultimately, the proposed work aims to use this population level heterogeneity to predict long term population dynamics across various biological systems.

It is anticipated in FY18 that the PI will determine the effects of local clustering of biomechanically similar cellular phenotypes in heterogeneous tissue environments on cancer incidence and tumor growth within the tissue environment. This is of interest as recent advances in cancer mechanobiology have highlighted to role of changes in cellular and extracellular mechanical properties on individual cell migration and proliferation dynamics. It is anticipated that integrating these observations within the proposed mathematical models of heterogeneous tissue environments will provide a biophysical understanding tissue dynamics and the early stages of cancer occurrence. Another expected outcome is a correlation between local vs global heterogeneity within a healthy tissue environment and the likelihood of cancer occurrence which could be then used as an early stage disease marker. These results will be validated against experimentally measured heterogeneity within cells of non-cancerous, malignant and metastatic tissue environments. This work and consequent validation will provide the platform for studying other tissue level processed such as wound healing, regeneration and aging.

D. Thermodynamically Constrained Averaging Theory for Multiscale Systems
Professor Cass Mill, University of North Carolina at Chapel Hill, Single Investigator Award

There is a standard model for two-fluid flow in porous media that is used in many different scientific fields. One aspect of this standard model is an empirical closure relation that relates fluid pressures and saturation; this is well-known to require history-dependent to describe real systems with even minimal fidelity. The field has not advanced past this; for example, a paper was published in 1980 on such an empirical relation, one of the most highly cited papers in the geosciences, and it was cited 1441 times in just the last year. A recent result of the current project based upon mathematical topology that shows that the state of the art empirical relation is poorly founded and is doomed to be hysteretic. An objective of this research is to replace this standard model with a much more mathematically rigorous model that is scale consistent that is able to describe how the system can be reformulated to remove the hysteresis. Success will need to demonstrate that the new form holds for a wide range of systems, vetted by the community of international collaborators. The standard closure relation requires a state history at every reversal point.

In FY18, it is anticipated that the employment of a Minkowski functional can be rigorously showed to eliminate the need for any history. This will rely on a unique relationship among a volume measure, an area measure, a mean curvature, and a Gaussian curvature, or equivalently on the Euler characteristic. Since this relationship is topological, therefore it would hold for any state, not just for an equilibrium state.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Joseph Myers
Division Chief
Program Manager, Computational Mathematics
Program Manager (Acting), Probability and Statistics

Dr. Virginia Pasour
Program Manager, Biomathematics

Dr. Leonard (Jay) Wilkins
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Dr. Andrew Vlasic
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B. Directorate Scientists

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C. Administrative Staff

Ms. Debra Brown
Directorate Secretary

Ms. Diana Pescod
Administrative Support Assistant

CHAPTER 9: MECHANICAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2017* is to provide an annual historical record summarizing the programs and basic research supported by ARO in FY17. ARO's mission is to support creative basic research resulting in new science that enables new materials, devices, processes, and capabilities for the current and future Soldier. This chapter provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions enabled by the ARO Mechanical Sciences Division in FY17.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Mechanical Sciences Division supports research to uncover fundamental properties, principles, and processes involved in fluid flow, solid mechanics, chemically reacting flows, explosives and propellants, and the dynamics of complex systems of relevance to the Army and the DoD. More specifically, the Division supports basic research to uncover the relationships to: (i) contribute to and exploit recent developments in kinetics and reaction modeling, spray development and burning, (ii) gain an understanding of extraction and conversion of stored chemical energy, (iii) develop a fundamental understanding that spans from a material's configuration to a systems response to create revolutionary improvements through significant expansion of the mechanical design landscape used to optimizing systems, (iv) developing innovative frameworks for analyzing and shaping the physical mechanisms and dynamical interactions underlying the control of nonlinear behavior in extended dynamical systems; embodied and distributed sensing, actuation, and control for robotic manipulation and mobility; and nonlinear topological mechanics of novel meta-structures; and the interplay between statistical physics and control and learning, (v) provide the basis for novel systems that are able to adapt to their environment for optimal performance or new functionality, and (vi) develop a fundamental understanding of the fluid dynamics underlying Army systems to enable accurate prediction methodologies and significant performance improvement, especially with regard to unsteady flow separation and flows characterized by fundamental non-linearities. Fundamental investigations in the mechanical sciences research program are focused in the areas of solid mechanics; complex dynamics and systems; propulsion and energetics; and fluid dynamics. Special research areas have been continued in the Army-relevant areas of rotorcraft technology, projectile/missile aerodynamics, gun propulsion, diesel propulsion, energetic material hazards, mechanics of solids, impact and penetration, smart structures, and structural dynamics.

2. Potential Applications. Research managed by the Mechanical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO research in the mechanical sciences could provide understanding that leads to insensitive munitions, tailored yield munitions, enhanced soldier and system protection, novel robotic, propulsion, and novel flow control systems and enhanced rotorcraft lift systems. In addition, mechanical sciences research may ultimately improve Soldier mobility and effectiveness by enabling the implementation of renewable fuel sources and a new understanding of energetic materials with improved methods for ignition, detonation, and control.

3. Coordination with Other Divisions and Agencies. The primary interactions of this Division with other ARL S&T Campaigns are with the Sciences for Maneuver, Sciences for Lethality and Protection and Materials Research Campaigns. The Division's research portfolio also supports the ARL ERAs of (i) Impact of Operating in a Contested Environment, and (ii) Implementation. The Division also interacts with the U.S. Army Corps of Engineers (USACE), and various Army Research Development and Engineering Centers (RDECs), including the Aviation and Missile RDEC (AMRDEC), Natick Soldier RDEC (NSRDEC), and the Tank-Automotive RDEC (TARDEC). The Division facilitates the development of joint workshops and projects with Program Executive

Office (PEO) Soldier and the Army Medical Research and Materiel Command (MRMC). In addition, the Division often jointly manages research through co-funded efforts with the ARO Chemical Sciences, Materials Science, Mathematical Sciences, Computing Sciences, and Life Sciences Divisions. Strong coordination is also maintained with other Government agencies, such as the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the National Science Foundation (NSF), the National Aeronautics and Space Administration (NASA), the National Institute of Standards and Technology (NIST), and the Department of Energy (DoE). International research is also coordinated through the International Science and Technology (ITC) London and Pacific offices.

B. Program Areas

The Mechanical Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of projects. In FY17, the Division managed research within these four Program Areas: (i) Solid Mechanics, (ii) Complex Dynamics and Systems, (iii) Propulsion and Energetics, and (iv) Fluid Dynamics. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Solid Mechanics. The goal of the Solid Mechanics Program is to investigate behavior of complex material systems under broad range of lading regimes in various environments, and to develop analytical and computational methods to characterize material models and to serve as physically-based tools for the quantitative prediction, control, and optimization of Army relevant material systems subjected to extreme battlefield environments. Army systems are frequently limited by material strength and failure resistance. Solid mechanics research plays a crucial role in the development of new materials, prediction of strength, toughness and potential damage development and failure of Army material systems, structures and individual protective equipment under extreme loading conditions such as impact or blast, and prolonged normal operating conditions. Research in analytical, computational and experimental solid mechanics forms the foundation of optimization tools to enhance performance while minimizing equipment weight, and its theories provide a strong link between the underlying mechanical behavior of solids and the resulting design and functionality of actual systems resulting in reduced development cost by minimizing the need for expensive field testing and it leads to novel ideas and concepts for revolutionary capabilities.

This Program Area is divided into two research Thrusts: (i) Investigation of mechanical behavior of complex material systems, and (ii) Development of analytical, computational and experimental methods capable to utilize material models in the analysis of extreme situations leading to damage and failure development. Current program efforts utilizing advanced multiscale computational and modeling techniques enabling detailed investigations of behavior of heterogeneous solids. The goal is to extend the design envelope of current and future Army structures, to develop predictive capability based on advanced ideas and understanding of material behavior across all relevant scales, to predict continuum and localized damage and failure initiation and development as it progresses across different scales, to give reliable estimates of the material limitations and useful life.

Research in this Program Area is focused on long-term, high risk goals that strive to develop the underpinnings for revolutionary advances in military systems. It is developing the methods needed to take advantage of recent advances in new materials fabrication and investigation technology, including nanotubes, nano-crystaline solids, and bio-inspired and hierarchical polymeric- and nano-composites. As a result of the long-term vision of the program, some future applications are not yet imagined while others will lead to the creation of ultra-lightweight, high strength materials for applications such as lightweight armor.

2. Complex Dynamics and Systems. The goal of the Complex Dynamics and Systems Program Area is to develop innovative frameworks for analyzing and shaping the physical mechanisms and dynamical interactions underlying the control of nonlinear behavior in extended dynamical systems; embodied and distributed sensing, actuation, and control for robotic manipulation and mobility; nonlinear topological mechanics of novel meta-structures; and the interplay between statistical physics and control and learning. In addition, the program has developed a set of Strategic Program Challenges (SPC) targeting questions relevant to the programmatic scientific focus areas deemed beyond the scope of single investigator awards. Current SPC topics include: (1) Energetic Versatility of Muscles: Principles and Emulation, (2) Controlling Hyperelastic Matter, (3) Theory of Morphological Energetics, (4) Control and Creation of Critical Dynamics, and (5) Nonlinear Topological Dynamics of Metastructures. The challenges emphasize high-risk, high-reward exploratory research to create breakthroughs, push science in truly novel directions, or to support mathematical abstractions and precise physical foundations for emerging technologies deemed likely to be of significant future Army and DoD impact. SPC's are developed by the program manager in close consultation with DoD researchers and university researchers.

The Complex Dynamics and Systems Program emphasizes fundamental understanding of the dynamics, both physical and information theoretic, of nonlinear and nonconservative systems as well as innovative scientific approaches for engineering and exploiting nonlinear and nonequilibrium physical and information theoretic dynamics for a broad range of future capabilities (e.g. novel energetic and entropic transduction, agile motion, and force generation). The program seeks to understand how information, momentum, energy, and entropy is directed, flows, and transforms in nonlinear systems due to interactions with the system's surroundings or within the system itself. Research efforts are not solely limited to descriptive understanding, however. Central to the mission of the program is the additional emphasis on pushing beyond descriptive understanding toward engineering and exploiting time-varying interactions, fluctuations, inertial dynamics, phase space structures, modal interplay and other nonlinearity in novel ways to enable the generation of useful work, agile motion, and engineered energetic and entropic transformations. The programmatic strategy is to foster mathematically sophisticated, interdisciplinary, and hypothesis-driven research to elucidate classical physics and analytical methods pertinent to the foundations of a broad spectrum of Army research areas including: mobility, power and energy, sensors, lethality, and trans-disciplinary network science.

3. Propulsion and Energetics. The goal of this Program Area is to explore and exploit recent developments in kinetics and reaction modeling, spray development and burning, and current knowledge of extraction and conversion of stored chemical energy to ultimately enable higher performance propulsion systems, improved combustion models for engine design, and higher energy density materials, insensitive materials, and tailored energy release rate. Research in propulsion and energetics supports the Army's need for higher performance propulsion systems. These systems must also provide reduced logistics burden (lower fuel/propellant usage) and longer life than today's systems. Fundamental to this area is the extraction of stored chemical energy and the conversion of that energy into useful work for vehicle and projectile propulsion. In view of the high temperature and pressure environments encountered in these combustion systems, it is important to advance the current understanding of fundamental processes for the development of predictive models as well as to advance the ability to make accurate, detailed measurements for the understanding of the dominant physical processes and the validation of those models. Thus, research in this area is characterized by a focus on high pressure, high temperature combustion processes, in both gas and condensed phases, and on the peculiarities of combustion behavior in systems of Army interest.

To accomplish these goals, the Propulsion and Energetics Program Area has two research Thrusts: (i) Hydrocarbon Combustion, and (ii) Energetics. The goal of the Hydrocarbon Combustion Thrust is to develop novel, predictive models for reacting systems especially for heavy hydrocarbon fuels, surrogate fuel development, and research into sprays and flames, especially ignition in high pressure low temperature environments. In addition the Energetics Thrust focuses on novel material performance via materials design and development and materials characterization, and investigations (theoretical, modeling and experimental) into understanding material sensitivity (thermal and mechanical).

4. Fluid Dynamics. Fluid dynamics plays a critical role in many Army operational capabilities. Significant challenges exist for accurate and efficient prediction of flow physics critical for improved performance and future advanced capability. Army platforms are often dominated by flows with high degrees of unsteadiness, turbulence, numerous and widely separated spatio-temporal scales, and geometrical complexity of solid or flexible boundaries. In order to gain the necessary physical insight to enable future capabilities spanning Army vehicles, munitions, medical devices, and logistics, the Fluid Dynamics program seeks to support basic research investigations of fundamental and novel flow physics. In view of the nonlinear and high-dimensional character of the governing equations, revolutionary advances in fluid dynamics research tools are also of great interest; advanced experimental methods, sophisticated computational techniques and breakthrough theoretical advances will be critical for gaining the required fundamental understanding.

Operating conditions for many Army platforms are characterized by flows featuring unsteadiness, nonlinear interactions, turbulence, three-dimensionality and flow separation. All efforts in this thrust area require novel and aggressive strategies for examination of the interplay between disparate spatio-temporal scales, inclusion of physically significant sources of three-dimensionality, and characterization of the role of flow instabilities and nonlinear interactions across a range of appropriate Mach and Reynolds numbers. Shortcomings in understanding the details of unsteady flow separation, reverse flow phenomena, and dynamic stall continue to limit the capabilities of Army rotorcraft vehicle platforms. While much progress has been made towards unraveling these details, it has become apparent that revolutionary advances are unlikely if the full complexity of the physics is not considered. Finally, many Army relevant flows are governed by strong nonlinearities and turbulent behaviors. Historically, many analysis tools developed for linear dynamics have been applied to gain understanding of flow behaviors. While local insights can be gained through applications of these methods, the ability to provide global understanding of the evolution of flows requires new approaches that are capable of dealing directly with inherent nonlinearities.

C. Research Investment

The total funds managed by the ARO Mechanical Sciences Division for FY17 were $15.9 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY17 ARO Core (BH57) program funding allotment for this Division was $8.3 million and $1.4 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $5.2 million to projects managed by the Division. The Division also managed $0.3 million of Defense Advanced Research Projects Agency (DARPA) programs. In addition, $1.4 million was provided for awards in the Historically Black Colleges and Universities and Minority Serving Institutions (HBCU/MSI) Programs, including funding for DoD-funded Partnership in Research Transition (PIRT), DoD-funded Research and Educational Program (REP) projects, and $0.7 million of the Division's ARO Core (BH57) funds, with the latter included in the BH57 subtotal above.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY16 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY17 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY17, the Division awarded 20 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Yuri Antipov, Louisiana State University; *Rapid Penetration of Rigid Bodies Into Elastic Media: Temperature, Boundary And Nonuniform Speed Effects*
- Professor Weinong Chen, Purdue University; *Damage and Temp around a Propagating Dynamic Crack*
- Professor Derek Dunn-Rankin, University of California - Irvine; *Ballistic Holography under Realistic Spray Conditions*
- Professor James Gregory, Ohio State University; *Unsteady Aerodynamics - Unsteady Compressibility Effects for Modern Rotorcraft*
- Professor Ronald Hanson, Stanford University; *Kinetics Fuels Using Shock Tube/Laser Absorption Methods*
- Professor Sinan Keten, Northwestern University Evanston Campus; *Engineering Nanocellulose Materials for High Ballistic Impact Performance*
- Professor Dennis Kochmann, California Institute of Technology; *Nonlinearity beats Damping: A New Class of Soft Active Metamaterials*
- Professor Henry Hess, Columbia University; *Thermodynamics of Learning*
- Professor Daniel Koditschek, University of Pennsylvania; *Morphological Computing in Machines and Animals*
- Professor Parisa Mirbod, Clarkson University; *Understanding the Instability of Particle-Laden Liquids Over Soft Porous Media*
- Professor Ahmed Naguib, Michigan State University; *Mechanisms of Force and Moment Generation by the Flow Over Oscillating Rectangular Cylinders*
- Professor Michelle Pantoya, Texas Technical University; *Surface Chemistry Promoting Energetic Material Combustion*
- Professor Steve Presse, Arizona State University; *Maximum Entropy as a Principle for Modeling Dynamics and Emergent Phenomena in Complex Systems*

- Professor Clarence Rowley, Princeton University; *Operator Methods for Analysis and Control of Dynamics, Networks, and Dynamic Networks*
- Professor Kunihiko Taira, Florida State University; *Characterization, Modeling, and Control of Turbulence from a Network-Theoretic Perspective*
- Professor Uwe Tauber, Virginia Polytechnic Institute & State University; *Control of Universal Scaling, Noise Strength, and Pattern Formation in Critical Dynamics*
- Professor Stephen Tse, Rutgers, The State University of New Jersey - New Brunswick; *Synthesis of Novel NanoEnergetics and Study of Their Reactant Interfaces*
- Professor Israel Wygnkanski, University of Arizona; *Fluidic Fences for Improved Aerodynamics of Rotating Systems*
- Professor Richard Yetter, Pennsylvania State University; *Experimental and Numerical Investigation of the Deflagration of Energetic Materials at High Pressures*
- Professor Minami Yoda, Georgia Tech Research Corporation; *Structured-Illumination Microscale Particle-Image Velocimetry*

2. Short Term Innovative Research (STIR) Program. In FY17, the Division awarded three new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Weinong Chen, Purdue University; *Impact Energy Dissipation through Force Chain Interruption*
- Professor Jack Edwards, North Carolina State University; *Mesh-sequenced Realizations for Evaluation of Subgrid-Scale Models for Turbulent Combustion*
- Professor Nicholas Gravish, University of California - San Diego; *Dynamical templates for sub-milligram legged locomotion*

3. Young Investigator Program (YIP). In FY17, the Division awarded three new YIP projects to drive fundamental research in an area relevant to the current and future Army. The following PIs and corresponding organizations were recipients of new-start YIP awards.

- Professor Steven Brunton, University of Washington; *Uncovering Nonlinear Flow Physics with Machine Learning Control and Sparse Modeling*
- Professor Chen Li, Johns Hopkins University; *Towards Terradynamics of Dynamic Legged Locomotion in Complex 3D Terrains*
- Professor Michael Mueller, Princeton University; *Multi-Modal Turbulent Combustion under Autoignitive Conditions: Separability of Combustion Modes and Implications for Modeling*

4. Conferences, Workshops, and Symposia Support Program. The Division provided funds in support of a range of scientific conferences, workshops, and symposia that were held in FY17. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences, with the goal of supporting scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army, and to define the research needs, thrusts, opportunities, and innovation crucial to the future Army. Proposals requesting funding support, typically for less than $10K, were received and evaluated in line with the publicly available ARO BAA. In FY17, four proposals were selected for funding by the Division to support FY17 conferences, workshops, or symposia.

5. Special Programs. In FY17, the Division also awarded eleven new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school and undergraduate students. These efforts were funded through the ARO Core Program and Youth Sciences Programs, for research to be performed at academic laboratories currently supported through active SI awards (refer to CHAPTER 2, Section IX).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Nanoscale Control, Computing, and Communication Far-from-Equilibrium. One MURI in this topic area began in FY13. The team is led by Professor James Crutchfield of the University of California at Davis. The objective of this MURI is to develop fundamental understanding to enable new synthetic nanoscale systems capable of behaving as information engines, performing tasks that involve the manipulation of both information and energy. Ultimately, a unified framework for understanding, designing, and implementing information-processing engines will be developed by a team of experts in information processing by dynamical systems, nonequilibrium thermodynamics, control theory, and nanoscale devices to search for and articulate the basic principles underlying the manipulation of information and energy by synthetic nanoscale systems. Theoretical predictions will be empirically validated in experimental nanoscale devices.

This research will enable new capabilities to (i) quantify the intrinsic computation in nanoscale thermodynamic systems, (ii) to produce a thermodynamic theory for control and optimization of out-of-equilibrium nanoscale processes, and (iii) to accomplish experimental validation of the resulting thermodynamic principles of optimization and control of molecular agents. The results will provide a scientific foundation for future nanoscale devices with groundbreaking capabilities, ranging from efficient computation on microscopic substrates to the generation of directed motion. In the long term, this research may enable devices that can coordinate the molecular assembly of materials and novel substrates for information processing on radically smaller and faster scales. This research may lead to a new generation of faster, cheaper, and more energy efficient computing devices capable of manipulating large-scale, complex data structures, as well as self-organizing nanoscale motors capable of interfacing with the physical world with maximum power and efficiency.

2. New Theoretical and Experimental Methods for Predicting Fundamental Mechanisms of Complex Chemical Processes. This MURI began in FY14 and was awarded to a team led by Professor Donald Thompson of the University of Missouri, Columbia. The objective of this MURI is to develop new approaches to predictive models for complex, reacting systems. It will develop supporting fundamental theory, perform supporting experiments, and validate resultant models and methods. The goal is to develop computationally efficient, predictive, accurate, robust methods to predict the molecular energy hypersurface, as well as relevant pathways and bifurcation topology for reacting coordinates.

The effort will accomplish the objectives via a comprehensive research program that will design efficient methods to predict and control the behavior of complex chemical reactions, such as combustion. Complexity is the salient challenge facing modern physical chemistry, and the proposed research will yield fundamental new methods to directly address the complexity of chemical reactions - from ab initio principles to the collective evolution of chemical populations. The research program is based on two ideas: (i) It is not necessary to describe or even know all the details, only those directly involved in the relevant pathway(s) from reactants to products, and (ii) it is essential to understand the role of fluctuations in the reaction rate, such as those that can be induced by the energetic environment and the many intermediates in combustion processes. The robust and accurate methods developed will determine the critical, emergent behaviors of complex overall reactions in non-equilibrium environments. They will accurately describe how a set of reactants undergoes sequential, branching reactions, passing through many transition states and transient species, to reach a final set of stable products. To gain an understanding of the role of fluctuations in reaction rates far from equilibrium, the researchers will focus on extracting information from the detailed dynamics of molecular species that are responsible for the fluctuations and, ultimately, the limits of traditional chemical kinetics. A synergistic approach will be undertaken for these overarching challenges that integrates the full range of rigorous fundamental theoretical methods. The specific objectives of the project leverage the complexity of kinetic phenomena, which are typically nonlinear, stochastic, multi-dimensional, strongly coupled, and can persist far from equilibrium by extreme variations in intensive properties. Some of the sub-objectives will be to: (1) Fully leverage the predictive capabilities of state-of-the-art electronic structure theory. (2) Gain a better understanding of how complex chemistry occurs at a microscopic level over wide ranges of temperature and pressure. (3) Identify and control relevant dynamical variables that can be probed experimentally. (4) Elucidate the role of statistical fluctuations in energy and matter on chemistry by analyzing the underlying nonlinear dynamics and reaction networks. (5) Design tractable theoretical and computational methods with immediate experimental links and reduced dimensionality without diminishing predictive capabilities. (6) Formulate connections among complexity theories, nonlinear dynamics, network theory, and chemistry. (7) Seek kinetic control of chemical and energetic phenomena on a macroscopic (rather than microscopic) level using nonlinear dynamics, optimal control, large deviations, and network theory.

3. Emulating the Principles of Impulsive Biological Force Generation. This MURI began in FY15 and was awarded to a team led by Professor Sheila Patek of Duke University. The objective of this MURI is to establish a unified theory for understanding biological and engineered impulsive systems. The MURI team will approach the objective using a thermodynamic framework linked to impulsive performance. This will require integrating mathematical analysis, tests of biological impulsive systems, and synthesis of impulsive materials and mechanisms. The thermodynamic framework consists of five phases: (1) chemical energy conversion in cellular biological systems that potentially circumvent the force-velocity tradeoffs of actin-myosin muscle mechanisms; (2) actuation tuned to spring loading through novel engineering implementations and informed by analyses of muscular and cellular thermodynamics; (3) potential energy storage through a diversity of biological materials, scales and geometries to inform synthetic elastic design; (4) rapid conversion from potential to kinetic energy (power amplification) – a defining feature of impulsive systems – through analyses of rate-dependence in biological materials/geometries, the mechanics of biological linkages and latches, and their directed synthesis into novel impulsive designs; and, (5) environment-system interactions through rigorous tests of the effects of environmental substrates and geometries, internal dissipation and reset mechanisms for repeated use and mitigation of failure due to environmental forces. This research effort will lay the foundations for scalable methods for generating forces for future actuation and energy storing structures and materials.

4. Multi-modal Energy Flow at Atomically Engineered Interfaces. This MURI began in FY16 and was awarded to a team led by Professor Jon Paul Maria of the North Carolina State University. The objective of this MURI is to bring chemistry, materials, surface science, electrochemistry, and physics together to characterize and understand short time-frame sub-nanoscale non-equilibrium phenomenon at and across materials interfaces, especially the flow, redistribution and partition of energy near the interface by devising and applying novel experimental, theoretical, and simulation approaches. This research is co-managed between the Mechanical Sciences (lead) and Chemical Sciences Divisions.

The MURI team approach will be to explore, identify, and define multiple mechanisms of energy transfer/transduction at precision-engineered interfaces. Material systems that support energy transfer through lattice/molecular vibrations, plasmon-electron coupling, and chemical reactions will be studied. The synthesis, measurement, and modeling activities are co-designed to promote extreme-non-equilibrium excitations within nano-scale geometries; to observe in situ picosecond to microsecond property responses using newly developed methods; to inform new theoretical models; and to enable accurate multiscale prediction. The plan of work explores a simple, overarching, and materials-generic hypothesis: function and failure in advanced functional materials are overwhelmingly affiliated with interfaces, where the underlying mechanisms (desirable and undesirable) are regulated by or related to energy transfer/ transduction among inhomogeneous boundaries. Observing and understanding the local processes over multiple time and length scales will improve existing and design new materials systems, and to predict their performance.

5. Data-Driven Operator Theoretic Schemes to Prediction, Inference, and Control of Systems. This MURI began in FY17 and was awarded to a team led by Professor Igor Mezic of the University of California at Santa Barbara. The objective of this MURI is to develop a spectral decomposition theory that encompasses elements of ergodic theory, geometric theory of dynamical systems, and functional analysis via the spectral theory of linear infinite dimensional operators, control theory, machine learning for inference, prediction and uncertainty analysis.

The MURI team approach will be to study systems in which there exists a model (e.g. the Navier-Stokes equation for fluid flow) as well as systems with no model (e.g. data streaming either from physical sensors or unstructured data). In both cases the team will develop efficient methods to extract the correct descriptive variables via spectral properties of associated operators. The main theory topics to be pursued will expand the current reach of spectral expansion analysis: 1) Stability theory for general attractors; treatment of continuous spectrum; 2) Uncertainty analysis and spectral expansion theory of the Perron-Frobenius operator for observable evolution; 3) Extensions to inference, prediction and control; 4) Spectral expansions for finite-time analysis; 5) Non-smooth systems. The main numerical analysis topics to be pursued will expand the current reach of spectral expansion analysis: 1) Proofs of convergence of finite-dimensional approximations to spectral objects of the infinite-dimensional Koopman and Perron-Frobenius operators; 2) Algorithms for finite-time analysis in nonautonomous and control systems; 3) Algorithms for extraction of finite-dimensional models from data for inference, prediction and control; 4) Rigorous utilization of machine learning algorithms in spectral expansion theory; 5) Utilization of spectral expansion theory for development of next-generation, real time computational tools for complex physics; applications to vortex dynamics. Finally, the team will investigate experimental and data analysis topics to expand the current reach of spectral expansion analysis: 1) Network monitoring problems arising in cybersecurity; 2) Experiments in locomotion for a class of hybrid oscillators; 3) Experiments on finite-time vortex stability; 4) Experiments on one of the most vexing continuous spectrum problems - turbulence in fluid-structure interactions leading to large deformations. All of these areas span DoD interests such as helicopter dynamics, robotics and cybersecurity. These developments in this MURI will lead to a massive changes in design, data inference, and control of systems possessing a very broad set of nonlinear features.

C. Small Business Innovation Research (SBIR) – New Starts

No new starts in FY17.

D. Small Business Technology Transfer (STTR) – New Starts

No new starts in FY17.

E. Historically Black Colleges and Universities / Minority Serving Institutions (HBCU/MSI) – New Starts

The HBCU/MSI program encompasses the (i) Partnership in Research Transition (PIRT) Program awards, (ii) DoD Research and Educational Program (REP) awards for HBCU/MSIs, and (iii) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). The Division did not have any new-start awards in this category in FY17; however, the Division continued to manage projects continuing from prior years.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY17.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY17, the Division managed 9 new DURIP projects, totaling $1.2 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. DARPA Reactive Material Structures Program

The Mechanical Sciences Division serves as the agent for the DARPA-sponsored Reactive Material Structures (RMS) program. This program was initiated in FY08 with an objective to develop and demonstrate materials/material systems that can serve as reactive high strength structural materials (*i.e.*, be able to withstand high stresses and can also be controllably stimulated to produce substantial blast energy). In FY13, Phase II of the program began, which continued and expanded research efforts. Research is investigating innovative approaches that enable revolutionary advances in science, technology, and materials system performance. The Mechanical Sciences Division currently co-manages projects in this program seeking to explore rapid fracture and pulverization of the material, dispersion of the particles, and material ignition and burning, all while achieving strength, density and energy content metrics. The vision of the RMS program is to be able to replace the inert structural materials currently used in munition cases with reactive material structures that provide both structural integrity and energy within the same material system along with the ability to rapidly release the energy upon demand.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Mechanical Sciences Division.

A. Impact with Material Comminution: New Concept - Turbulence Analogy

Professor Zdenek Bazant, Northwestern University, Single Investigator Award

The objective of this research is to develop a new model characterizing concrete response to a high rate strain loading. The model includes a shear strain rate dependent viscosity term leading to kinetic energy absorption during material fragmentation. This innovative step, hopefully, could be used in simulations and predict the effects of high strain rate impact, explosions and shock waves on concrete structures and other brittle materials. The current material behavior models consistently underestimate material resistance under the high rate impact loadings. To accomplish this objective, the energy dissipated by interface fracture of forming particles will be simulated by artificial equivalent shear viscosity, analogous to the viscosity enhancement by turbulence, which will be implemented in the material subroutine of a finite element program. A dimensionless indicator analogous to Reynold's number is to be introduced to delineate interface fracturing by release of kinetic and strain energies.

In FY17, the effort achieved several results towards the above objective. First, a kinetic fracture model was incorporated into the damage constitutive model. To achieve this, a strain-rate dependent microplane constitutive damage model was combined with the theory of dynamics comminution of concrete under impact at extreme strain rates (10/s—1,000,000/s), based on the theory of release of kinetic energy of the strain-rate field in forming particles. This model correctly simulates the so-called dynamic 'overstress'. The theory correctly predicts the sizes of comminuted particles and the part of kinetic energy that must be dissipated in the finite element code to match the observed projectile velocities, depths of penetration and entry and exit crater shapes. This kinetic energy is dissipated in computations by using a factor proportional to the -4/3 power of the strain rate to scale up the material strength in the microplane model. The model also has been extended to various angles of the impacting projectile, as well as materials of various strength and layered materials. The model is also capable of simulating and predicting lateral branching of cracks, which was not possible before.

As a side effort of the work, an examination of 'Peridynamics' was conducted as this is an often proposed tool for brittle fracture prediction and analysis: The relatively new approach, inspired by efficient computer codes for molecular dynamics, was proposed for the computational simulation of impact and explosion effects on concrete and rock structures, and heterogeneous quasibrittle materials in general. The conclusion is that while peridynamics is, under the hypotheses made, a mathematically rigorous and elegant looking approach, it is unsound from the physical and engineering viewpoints, for 5 reasons: 1) In similarity to molecular dynamics, the quintessential hypothesis of peridynamics is the existence of particle skipping interactions, i.e, a direct interaction of the central particle with its second, third, etc. members, by means of some hypothetical potential that has no physical basis. Such interaction is true only for atoms, but is physically incorrect on any higher scale. In reality, transmission of forces to the second and farther particles is mediated by displacements and rotations of the intermediate particles and relative displacements at particle interfaces. 2) In the elastic regime, peridynamics exhibits excessive wave dispersion, the state-based version more so than the bond-based version. 3) In the inelastic (plastic and damage) regimes, peridynamics cannot properly distinguish between wave dispersions due a) to material heterogeneity and to b) development of microcracks or microslips. 4) Peridynamics is a step backwards because the classical nonlocal or crack band models are better. They are better founded physically and give more realistic results. E.g., they can model the important case where dispersion due to heterogeneity is much weaker than dispersion due to inelastic phenomena in the meso-structure. 5) For damage of concrete and some rocks, the RVE is large enough in the typical case of laboratory specimens (in which no significant damage localization takes place). There are 21 different types of uni-, bi-, and triaxial tests of such specimens, monotonic and cyclic, proportional or noproportional of various kinds, available for characterizing concrete.

These tests have all been successfully fitted by advanced constitutive models such as the microplane model or Jirasek-Grassl model, and were used in model calibration. But peridynamics has never been fitted to these or similar data. It has been used to create realistically looking movies of structural failures with hardly little significant input from uni-, bi- and triaxial material testing.

B. Metastable Mechanical Modules: Inspiration for a New Class of Engineered Adaptive System

Professor Kon-Well Wang, University of Michigan, SI Award

The goal of this project is to develop a new class of adaptive structural/material systems that exhibit unprecedented levels and forms of versatility by elucidating and utilizing the multiscale mechanical principles of skeletal muscle. To achieve this goal, researchers are investigating structural/material systems that leverage metastability, modularity, and multi-dimensionality—characteristics observed in muscle architectures (see FIGURE 1). In addition, through the muscle-inspired structural mechanics studies, this research may provide opportunities to interpret the spectrum of mechanical principles underlying muscle energetics.

Three major accomplishments were achieved in FY17. First, researchers characterized the mechanics and energy capture behaviors of asymmetrical bistable modules and structures comprised of such modules. This direction built upon recent findings suggesting that skeletal muscle cross-bridges are responsible for a significant portion of the stored elastic energy in muscle. This energy is captured from inertial loads and used to enable rapid explosive motion, or improve the efficiency of periodic, cyclic movements. Inspired by this functionality and the asymmetric bistability expressed by the cross-bridge's power-stroke constituent, researchers studied the influence of energetic asymmetries on strain energy capture under quasi-static and impulsive loads. Results demonstrate up to 30% capture of initial energy as recoverable strain energy for the structure parameters under consideration, and reveal a balance between maximizing the amount of trapped energy and the onset of snap-back to low energy states with no energy capture. Since thermal noise strongly influences the mechanics of muscle sarcomeres and crossbridges, the effect of noise on the modular structure was studied. The addition of white noise was shown to greatly inhibit energy capture, with a maximum of 10% of inertial energy trapped for the parameters under consideration. Highly asymmetric structures exhibit no strain energy capture; suggesting that the degree of asymmetry should be strategically selected based on the expected noise magnitude.

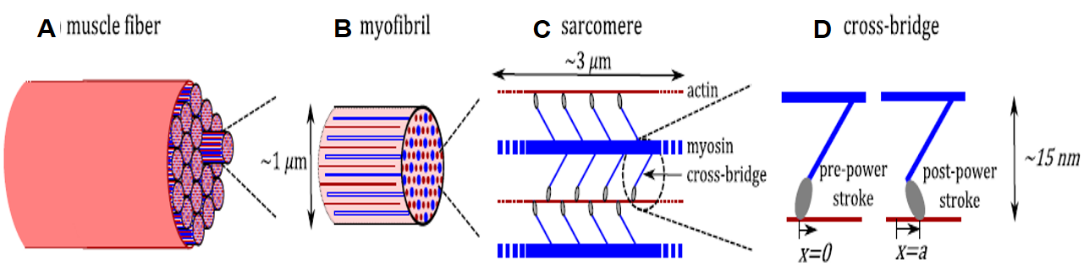

FIGURE 1

Muscle Architecture as Inspiration for Adaptive Structures. Muscle fibers (**a**) are composed of bundles of (**b**) myofibrils, which are sectioned into units called (**c**) sarcomeres. These sarcomere units consist of adjacent actin and myosin proteins, connected by (**d**) cross-bridges. Muscle's fundamental force generating process is the cross-bridge power stroke, which causes the actin and myosin filaments to slide against each other. The power stroke is influenced by the lattice spacing between adjacent filaments, which confines its mechanics in the direction transverse to the axis of fiber contraction.

Second, researchers explored the rich mechanics afforded by combining of multistability, metastability, and oblique motions. Across length scales, skeletal muscle exploits multidimensionality and the geometric relationships between its constituents to assist in force generation, dramatic length change, and energy storage. The lattice spacing and transverse confinements imposed on micro-scale sarcomere chains influences conformational changes associated with the power-stroke, which is the basic force generating unit of muscle. From a macroscopic perspective, certain muscles are composed of fibers with an oblique, pennate architecture to facilitate large motions while minimizing over-straining. Researchers found that the reaction force and energy profiles may be tailored by varying void geometry and wall thickness, as well as by the level of transverse confinement imposed on the module. Adaptability is enhanced by considering systems composed of multiple constituents. Experimental efforts carried out on silicone rubber specimens with circular voids demonstrate that transverse confinement influences multistability under oblique motions, with specimens exhibiting bistability or tri-stability based on the level of transverse confinement enforced. Experimental and numerical investigations of constituent four-void modules reveal the existence of metastability where different conformations exhibit significant variations in reaction force, stiffness, and strain energy. Discrete transitions between configurations corresponding to rapid releases of stored elastic energy enable dramatic changes in reaction force.

Third, researchers developed a novel approach to accomplish nonreciprocal wave propagation with exceptional adaptivity by exploiting the concept of metastable modular metastructures (see FIGURE 2). Reciprocity describes the symmetry of wave transmission between two points in space. If a wave can propagate from a source to a receiver, it is equally possible for the wave to travel in the opposite path, from the receiver to the source. Considerable efforts have been devoted to realize non-reciprocal behavior through linear systems with additional symmetry breaking mechanisms or directly through nonlinear systems. The new approach could foster a new generation of reconfigurable structural and material systems with non-reciprocal characteristics that are applicable to vastly different length scales for a wide spectrum of applications. Experimental efforts were begun wherein a bistable constituent is generated by press fitting three magnets with repulsive polarization inside a 3D printed enclosure connected in parallel with a stabilizing spring realized via spring steel. Numerical efforts have been performed on a chain of metastable modules, indicating that non-reciprocal energy transmission is facilitated by being able to trigger the onset of nonlinear supratransmission at different excitation levels for different opposite directions due to spatial asymmetry. Therefore, by intelligently leveraging nonlinearity, spatial asymmetry, periodicity, and ability to be reconfigured, the structure is endowed with the opportunity to on demand tune and control unidirectional wave propagation. By exploiting the programmable properties invested in the metastable modules and structure, unprecedented adaptivity of non-reciprocal wave transmission characteristics have been exemplified with internal reconfiguration and metastable state change, as input amplitude and frequency vary.

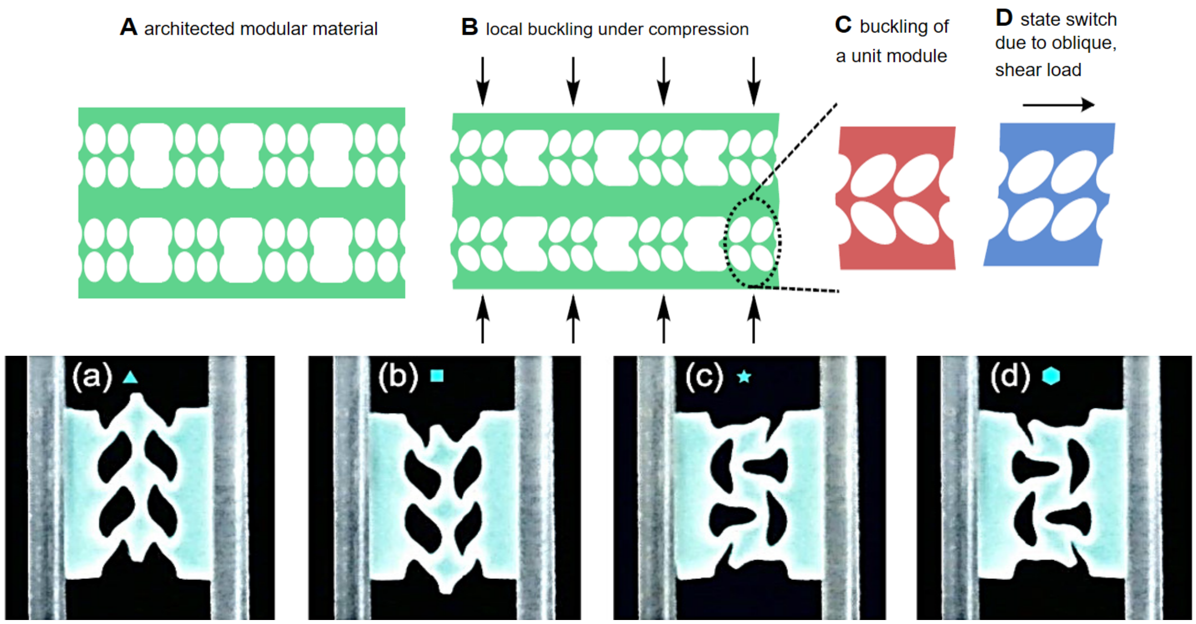

FIGURE 2

Structures Comprised of Metastable Modules. (Top) (A) Section of architected modular material system subject to compression (B), resulting in local buckling of constituent modules (C). Applying a shear load causes a discrete switch (D) in the void pattern. This illustration summarizes the research concept, where structural/material systems are composed of unit constituent modules that may exhibit multiple deformation and buckling modes under a variety of applied strains. (Bottom) Four different configurations for a four-void unit specimen under the same prescribed transverse confinement and global shear. Images (A) and (B) depict configurations where deformations of the voids are aligned in the same direction, while (C) and (D) depict polarized deformations of the voids. The samples are initially 30mm wide, and are subject to a 5.7mm compression in the transverse (horizontal) direction.

C. Interaction of an Underexpanded Supersonic Jet and a Compliant Surface

Professors J. Craig Dutton and Gregory Elliott, University of Illinois - Urbana-Champaign, Single Investigator Award, DURIP

The objective of this effort was to gain insight into the fluid-structure interaction (FSI) of an underexpanded sonic jet and a compliant surface adjacent to the jet nozzle. Jet/surface interactions have been commonly studied due to relevant real-word applications and the associated wide array of fluid dynamics phenomena. While jets flowing over nearby rigid surfaces has been studies to some degree (especially in the acoustics community), there is little known about the effect of surface compliance on the flow physics. Understanding the impact of compliance has potential relevance for mitigating jet screech in aerospace propulsion and airframe structural interaction issues.

During FY17, the research team completed simultaneous full-field measurements of fluid and structural states utilizing instrumentation obtained via an ARO-supported DURIP award. The flowfield was measured using Digital Particle Image Velocimetry (DPIV) and the structural response was measured using stereo Digital Image Correlation (sDIC), with an electronic timing system employed to manage the synchronization of the two systems. While this technique had been previously used by other researchers for low-speed flows, this study represents the first truly high-speed FSI measurements made in this manner. The measurements obtained were compared against previous measurements conducted on a rigid surface.

The surface was observed to have a response that was characterized by a deflected contour with a standing-wave pattern and was reasonably quasi-static. The region of the surface coincident with the first shock-cell featured a deflection towards the jet, while waves further from the jet were smaller in magnitude and predominantly directed away from the jet. The deflection of the compliant-surface induces a region of lifting-flow and a supersonic compression-expansion region in the first shock cell. This produces reduced inflow Mach numbers for the shock-boundary layer interaction (SBLI) region, and results in subsequent alterations of the shock structure (see FIGURE 3). These changes appear to result in a weaker shock system and increased SBLI-exit Mach numbers. Further, the compliant surface develops a substantially thicker wall boundary layer as compared to a rigid-surface.

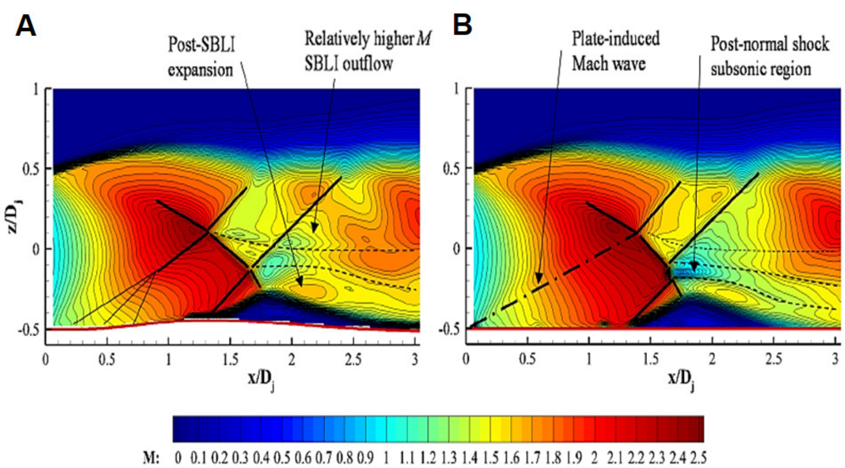

FIGURE 3

Shock structure alteration due to compliance. (**A**) Compliant surface, showing higher speed outflow and an expansion behind the SBLI relative to (**B**) the rigid surface. Color contours are Mach number.

D. Electrokinetic Instabilities for Manipulation and Self-Assembly of Nano/Microparticles

Professor Minami Yoda, Georgia Institute of Technology, Single Investigator Award

The objective of this research is to investigate the underlying physical mechanisms associated with the observation of the formation of bands of particles in combined Poiseuille and electro-osmostic flow through a microfluidic channel (see FIGURE 4). Under certain conditions, a dilute suspension of polystyrene particles flowing through a fused-silica channel will spontaneously assemble into periodic bands aligned with the flow (and the electric field) near the wall. The working hypothesis is that there exists an electrokinetic instability that results from a wall-normal particle concentration gradient, which then creates a gradient in the electrical conductivity / permittivity of the fluid. An experimental approach is being pursued, as there exists an absence of valid theoretical knowledge with which to explain the observations.

In FY17, experiments were performed for different suspension concentrations through a microfluidic channel, while also varying the strength of the pressure gradient (Poiseuille flow) and the dc electric field (electro-osmotic flow). Near-wall particles are imaged using evanescent wave visualization techniques (previously developed in part with support from an ARO STIR award and a DURIP award). The results suggest that band formation occurs only after the electric field magnitude increases above a threshold value. This threshold value is a function of the local shear rate, along with the particle diameter, ζ-potential, and concentration. The band formation is also an initially dynamic process, with band formation accelerating with increased shear rate and particle ζ-potential. The number and size of bands varies initially, but eventually reaches a steady state, with the number of bands also a function of the above parameters.

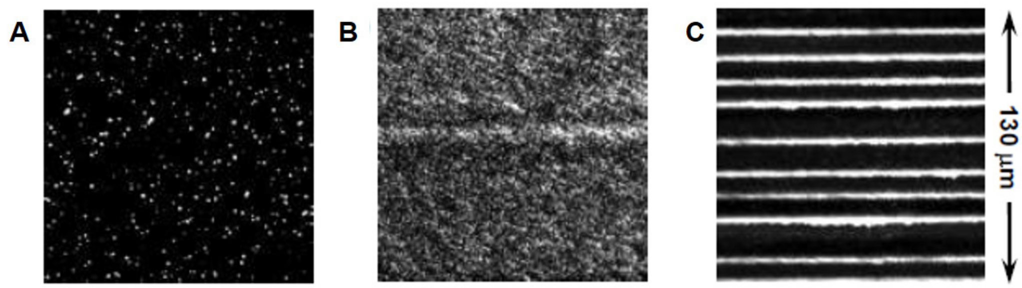

FIGURE 4

Band formation in a dilute suspension. Evanescent-wave visualizations of near wall particles (d = 245 nm) in (A) Poiseuille flow (near-wall shear 650 s^{-1}), (B) and combined with electro-osmotic flow (E = -28 V/cm) where bands are beginning to form, and (C) with fully formed bands (E = -70.7 V/cm). Poiseuille flow is to the right and the electro-osmotic flow is opposite. Only particles in the near wall region (~1% of channel depth) are visible.

Some initial modelling efforts were also undertaken, which predicted that near-wall reverse flow would occur; this was experimentally verified. The model also suggests that the combination of electric double layer and van der Waals forces dominate over other forces. Thus, particle and channel-wall surface properties likely play a major role in particle-particle attraction and subsequent band assembly. Continuing efforts will couple high-speed imaging and axial-plane optical microscopy in order to gain greater understanding of the governing particle dynamics; measurements of the particle-particle interactions, along with determining whether particles in the bands originate from the near-wall region or the bulk flow (or both). Experiments with heterogeneous particles will also be conducted to determine if control of surface ζ-potential will provide capability to regulate particle assembly for the creation of novel materials.

E. Fundamental Mechanisms of Impact Initiation of Reactive Materials

Professor Dana Dlott, University of Illinois - Urbana-Champaign, Single Investigator Award

The goal of this project is to understand the fundamental mechanisms of shock initiation of reactive materials (RM) or energetic materials (EM) using advanced shock compression instrumentation and diagnostics. The experiments in focus for this research are radically different from the usual shock compression techniques that involve using large guns or bombs as experiments are conducted on a tabletop under a microscope, and hundreds of shots can be conducted per day. Shocks can be studied with unprecedented detail and under a wide variety of conditions. The tabletop experiments produce planar shocks that are as powerful and as well-characterized as the most advanced gas gun systems. However the shocks are tiny, 0.5 mm in diameter, and the duration is short, less than 20 ns. While the method has limitations in that it cannot study large scale, long time phenomena such as the blast effects of a bomb, but it is ideal for understanding the short time-short length scale phenomena that reveal fundamental mechanisms. In particular the techniques allows understanding of shock initiation of RM and EM at the atomistic level and at the mesoscale level.

Results of recent studies shows the HMX studied reacts in two stages. The first stage starts near the end of the shock and it lasts for a few tens of nanoseconds. The second stage, which is a deflagration at ambient pressure, starts at a few hundred nanoseconds and lasts for 10 microseconds or more. In a unique HMX experiment, the impact velocity was held at 2.0 km/s while the shock duration was varied from 2.5 to 16 ns using Al foil flyers ranging from 12.5 to 75 micron thick (see FIGURE 5). This allows one to roughly map out chemical kinetics in the shock reaction zone. A two stage reaction in the emissivity is observed. As the shock duration increases, the faster part becomes bigger at the expense of the slower part. With longer-duration shocks, there is more time for the reaction during the shock and less unreacted material left over to feed the later deflagration. When the shock is short in duration, it interrupts the HMX shock reaction.

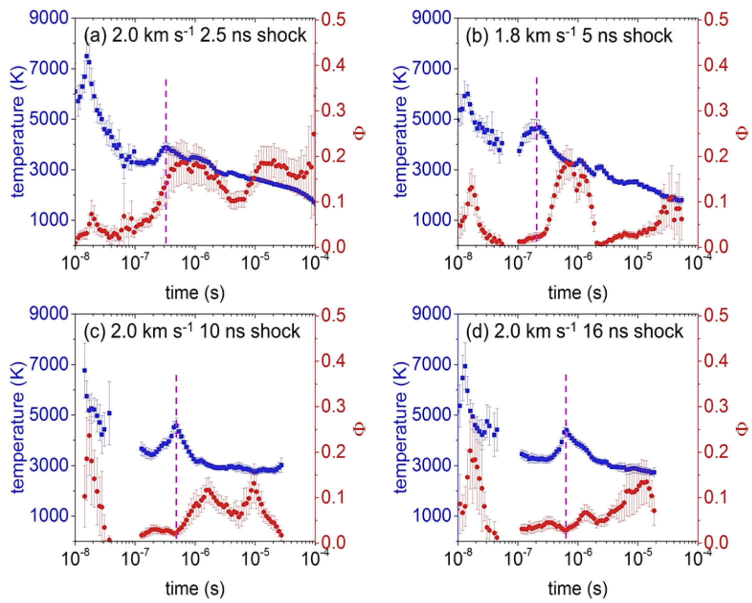

FIGURE 5

A series of shots on HMX at 2.0 km/s with different duration shocks. The emissivity shows a nanosecond and a microsecond process, representing two stages of chemical reactivity. With longer duration shocks, an increasing amount of the chemical reactivity happens in the nanosecond regime.

Subsequent experiments utilized a PBX quite similar to the commercially available PBX denoted XTX-8003 or simply "XTX". The XTX was made in two microstructural forms of a highly microporous structure. The microporous XTX is then compressed with a hydraulic press to squeeze out the pores. This compression step is also used in the synthesis of the commercial XTX. After compression, scanning electron microscope images show that there are no visible pores larger than 1 micron XTX is then compressed with nanoporous or homogenized XTX. Shock initiation of these two microstructures produces dramatically different results (see FIGURE 6). With the microporous XTX, the shock produces a massive concentration (a large emissivity change) of hot spots that reach more than 7000K. Then there is a slower process where the unreacted material deflagrates on the microsecond time scale.

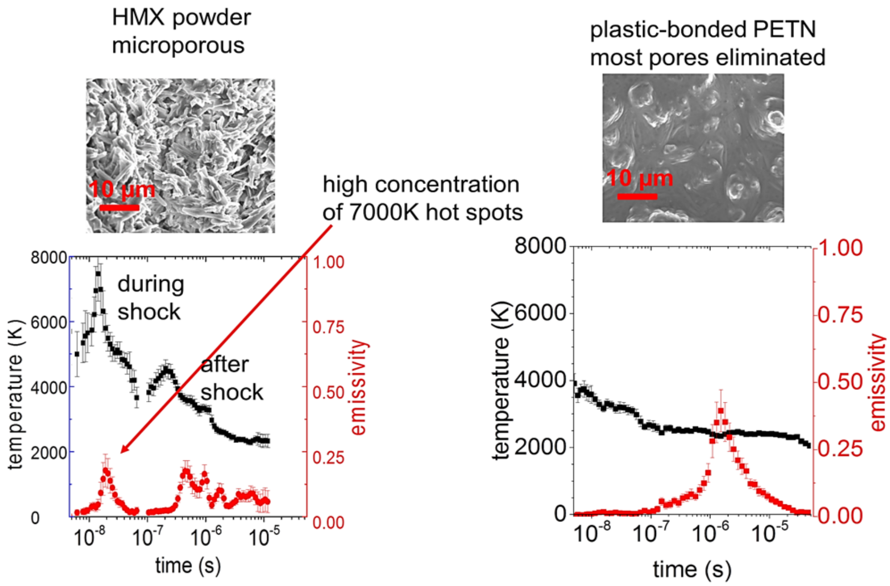

FIGURE 6

Experiments at 2.7 km/s on PETN-based plastic explosive XTX-8003 made either microporous or nanoporous. The microporous material has many hot spots up to 7000K. Homogenizing the material eliminates the hot spots and concentrates the reactivity into a narrow time range around 2 microseconds.

The massive concentration of hot spots produced in the microporous XTX results from adiabatic compression of gas in the pores. Gas compression produces much higher temperatures than solid compression due to the much larger volume change with gas. The temperature histories with 2.8 km/s impacts when the gas in the pores was air, Ar, N_2, O_2, C_2H_2 and C_4H_{10} are shown in FIGURE 7. The polyatomic gases make much lower initial temperatures than the monatomic and diatomic gases due to their higher heat capacities. This shows that the high temperature hot spots are created by gas compression. It is interesting that the same behavior is seen when the sample is in vacuum as when it is filled with polyatomic gases. The team found that when the sample is in vacuum, the shock causes the PETN to outgas and fill up the pores with polyatomic molecule gases. This means that experiments where people put the sample in vacuum do not really eliminate gas in the pores. The pores were promptly filled with gas produced by the explosive.

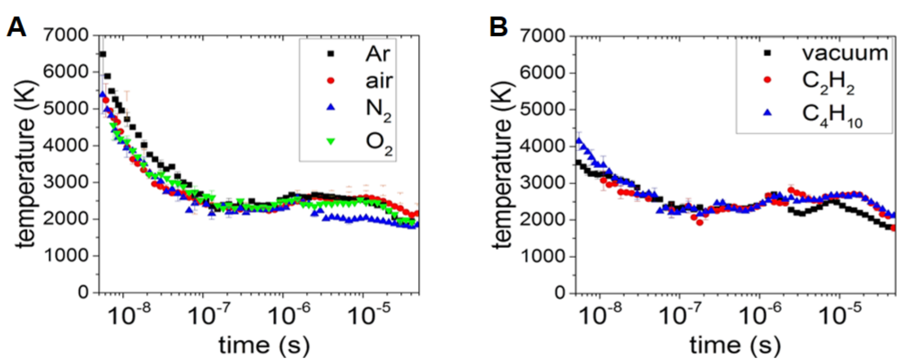

FIGURE 7

Temperature histories for XTX-8003 at 2.7 km/s with the pores filled with different gases. The peak temperatures are much lower with the polyatomic gases.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Advanced Large Eddy Simulation Methodologies for Industrial Flows

Investigator: Professor Z.J. Wang, University of Kansas, Single Investigator Award
Recipients: Advanced Rotorcraft Technology, General Electric Global Research

Large eddy simulation (LES) has been shown to be a promising tool for calculation of complex turbulent flows. Often, the computational costs associated with running such simulations render them of limited value for industrial design applications when high-order accuracy is required and when geometric complexity of the flowfield is high. Active research is currently working to address this limitation, developing methodologies that bring the costs for high-order simulations down to levels useful for industrial application. The current research effort focuses on the method known as flux reconstruction (FR) or correction procedure via reconstruction (CPR). This research effort led to the LES of a benchmark flow over a turbine blade at Reynolds numbers near 600,000, with good agreement with experimental data for mean surface skin friction and heat transfer.

A significant pacing item in employing high-order methods in real world flow simulations is high-order meshes, in which edges are represented by degree two or higher polynomials. This is because such simulations require "coarse meshes" relative to those used in second order methods. Linear meshes introduce solution errors near wall boundaries, which destroys the quality of the high-order solution. Advances in high-order meshing tools, coupled with the FR/CPR methodology and progress in modeling of both near-wall and dissipative physics, have allowed significantly more accurate results in comparable computational time. Researchers at GE Aviation and GE Global Research performed the same calculation using both FLUENT (a commercially available code with second order accuracy) and FDL3DI (a high-order code developed by the Air Force). As expected, the high-order codes resolve much more significant flowfield detail than the second order code. The main advantage of the new methodology is the utilization of an unstructured mesh, which permits an order of magnitude decrease in mesh generation time and significantly improved scalability for large-scale parallelization. GE Global Research licensed the code and adopted it as their standard LES formulation.

B. Dynamic Stall Reduced Order Modeling for Real-Time Flight Simulation

Investigators: M. Smith, Georgia Tech and D. Peters, Washington University, Single Investigator Award
Recipient: Advanced Rotorcraft Technology

Dynamic stall is a critical performance limiting phenomena for rotorcraft vehicle platforms. As the forward flight speed of a helicopter increases, the aerodynamic loading on the rotor blade increases to a point where the boundary layer separates over a portion of the blade across a short range of azimuthal angles. This separation event generates a complex vortex system, which leads to highly unsteady forces and moments and results in vibrations that cause component failure. In spite of the fact that dynamic stall is a "well-known" phenomena, its onset and impact on flight qualities is still very difficult to predict.

Researchers at the Georgia Institute of Technology conducted high-fidelity computational investigations to uncover underlying mechanisms of the dynamic stall event. A collaboration with researchers at Washington University led to the development of reduced-order models that reproduce many of the important forces and moments. These models include many important effects, such as the influence of a time-varying freestream and spanwise flow effects (capturing 3D details). ART has incorporated these reduced-order models into both the Rotorcraft Comprehensive Analysis System (RCAS) and FLIGHTLAB. RCAS provides comprehensive aeroelastic analysis of rotorcraft vehicle systems, including structural dynamics, aeroelastic stability, vibration, and loads prediction. FLIGHTLAB is a finite element, component-based, selective fidelity modeling and analysis software that enables real-time prediction of rotorcraft performance for use in simulated environments. Greater fidelity of simulation permits both increased capability to test conceptual vehicles, as well as provide pilot training on dynamic stall mitigation for rotorcraft currently in service.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Damage and Temperature around a Propagating Dynamic Crack

Professor Weinong Chen Purdue University, Single Investigator Award

The goal of this research is to develop methods and methodologies to visualize the damage and temperature fields in real time around a propagating crack tip. This will be achieved through several methods, including, visualizing the crack tip damage field evolution in real time using high-speed X-ray phase contrast imaging and measuring the temperature field evolution using a laser-induced phosphorescence method. Materials under study will include a glassy polymer and a metallic. To vary the dynamic loading rates, the crack will be driven by a Kolsky bar and a light gas gun. The temperature field will be measured with a new 2D topographical temperature measurement method using the laser-induced phosphorescence of embedded or coated particles providing continuous temperature measurements. High-speed measurement of the dynamic temperature field around the crack initiation and propagation region will be achieved using laser-induced phosphorescence (LIP). In FY18, this project will develop the imaging methods and complete the first dynamic fracture experiments with damage visualization for several materials with crack growth driven by the Kolsky bar setup.

B. Characterization, Modeling and Control of Turbulence from a Network-Theoretic Perspective

Professor Kunihiko Taira, Florida State University and Professor Steven Brunton, University of Washington, Single Investigator Award

The objective of this research is to perform network-based characterization and modeling of turbulent vortical interactions and utilize the findings to implement network-based control of canonical turbulent flows. Further, analyzing the effects of random and focused actuations on the vertical network nodes will motivate studies towards exploring the resilience of the network. Also, identifying the important coherent structures or communities in the network will help formulate reduced-order models for the dynamics of the fluid flow.

The research approach includes (1) characterization of time-varying turbulence networks and develop sparsified low-order models, (2) investigation of a hierarchy of models of increasing complexity, (3) explore network resiliency to random and focused actuation at vortex “hubs,” (4) infer network interactions and develop balanced reduced-order models of dynamics from turbulence fluid flow data, and (5) perform network-based open and closed loop control of turbulent dynamics.

Currently, the majority of the effort has focused on 2D turbulent networks. In FY18, it is anticipated that the characterization of 3D turbulence will be performed, using the generalized Biot-Savart law to define the network interactions. Modeling of the flow dynamics will be performed using a reduced network representation, employing intelligent model reduction and sparsification techniques. It is also expected that analyses will reveal which turbulent structures have the largest overall impact on the flow evolution, which will form the basis for eventual control strategies.

C. Towards Terradynamics of Dynamic Legged Locomotion in Complex 3D Terrains

Professor Chen Li, Johns Hopkins University, Single Investigator Award

The objective of this research is to lay the foundations for a terradynamics of legged locomotion in complex spatial terrains (e.g. dense vegetation, randomly scattered obstacles, rubble) by casting the problem as one of motion in a fluctuating energy landscape and using methods from statistical mechanics to characterize the distribution of movement in complex terrains. It is anticipated that in FY18 the PI will test the hypothesis that vibrations and perturbations from locomotor-terrain interaction during legged locomotion serve as “energy fluctuations” to allow the formation of locomotor pathways. The crux of the approach is inspired by free energy landscapes that allow understanding of the statistical distribution of protein-folding pathways brought about by thermal fluctuations. Preliminary locomotion energy landscape models indicate that movement is statistically more probable via locomotor pathways that overcome lower energy barriers in a manner analogous to equilibrium systems being more likely to occupy lower energy states. However, while locomotor systems are instead far-from-equilibrium, recent studies suggest that dissipative forces in complex 3D terrains may be comparable to self-driving forces from appendages, resulting in "non-inertial" properties of the total locomotor-terrain interaction system (see FIGURE 8). To test the hypothesis, the PI will focus on four research areas: (1) Creation of new terrain devices to partition and parameterize complex 3-D terrains, (2) Animal experiments to measure locomotor performance and pathways, (3) Robophysics experiments to vary locomotor and terrain parameters to discover general principles, and (4) Statistical mechanical modeling to understand formation of locomotor pathways.

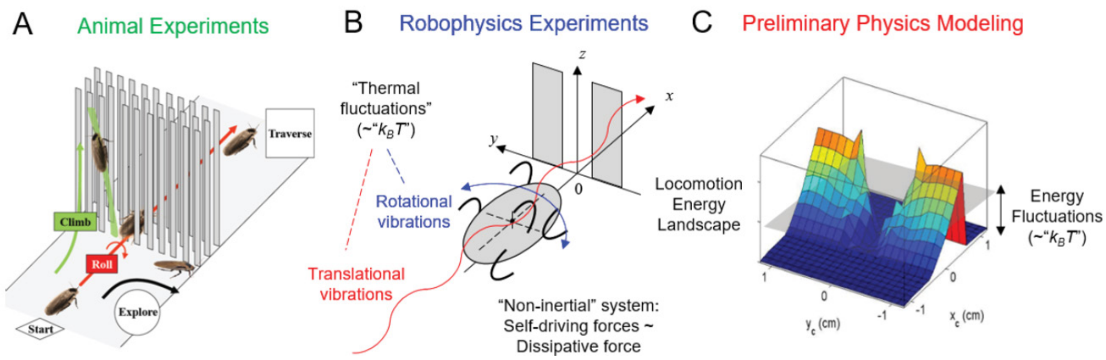

FIGURE 8

Framework for terradynamics in complex 3D terrain. Recent research of beam obstacle traversal and preliminary modeling supports the vision that locomotion energy landscapes will allow understanding of the statistical distribution of movement in complex 3-D terrains.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Ralph Anthenien
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CHAPTER 10: NETWORK SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2017* is to provide an annual historical record summarizing the programs and basic research supported by ARO in FY17. ARO's mission is to support creative basic research resulting in new science that enables new materials, devices, processes, and capabilities for the current and future Soldier. This chapter provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions enabled by the ARO Network Sciences Division in FY17.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Network Sciences Division supports research to discover mathematical principles to describe, control, and to reason across the emergent properties of all types of networks (*e.g.*, organic, social, electronic) that abound all around us. The unprecedented growth of the internet, the tremendous increase in the knowledge of Systems Biology, and the availability of video from US military operations have all led to a deluge of data. The goal of the Network Sciences Division is to identify and support research that will help create new mathematical principles and laws that hold true across networks of various kinds, and use them to create algorithms and autonomous systems that can be used to reason across data generated from disparate sources, be they from sensor networks, wireless networks, or adversarial human networks, with the resulting information used for prediction and control. Given that network science is a nascent field of study, the Network Sciences Division also supports basic research on metrics that are required to validate theories, principals and algorithms that are proposed.

2. Potential Applications. Research managed through the Network Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO through network science research may provide new and revolutionary tools for situational awareness for the Solider and new regimes for command, control and communication for the Army. Furthermore, work supported by ARO through the Network Sciences Division could lead to autonomous systems that work hand-in-glove with the Soldier.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Network Sciences Division frequently coordinates and leverages research within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), and the Defense Advanced Research Projects Agency (DARPA). In particular, the Division's portfolio is coordinated with the ARL Information Science, Computing Science, and Human Sciences Campaigns by both influencing the development of Campaign strategies, and by being cognizant of the Campaigns' needs. The Division's research portfolio also supports the ARL ERAs of (i) Intelligent Teams, (ii) Impact of Operating in a Contested Environment, and (iii) Implementation.

In addition, the Division frequently coordinates with other ARO Divisions to co-fund research, identify multi-disciplinary research topics, and to evaluate the effectiveness of research approaches. For example, interactions with the ARO Computing Sciences Division include promoting research to investigate game-theoretic techniques that could lead to better cyber situational awareness and to address concerns about performance and resilience to cyber attacks in ad-hoc dynamic wireless networks in a uniform fashion. The Network Sciences Division also coordinates its research portfolio with the Mathematics Division to pursue studies of game theory that address bounded rationality and human social characteristics in a fundamental way. The Network Sciences Division coordinates with Life Sciences on studies at the neuronal level to understand human factors in how decisions are made under stress. Lastly, the Division's Program Areas interface with the Mechanical Sciences Division to understand the interplay between learning and manipulation and locomotion in robotic systems.

B. Program Areas

The Network Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY17, the Division managed research within these five Program Areas: (i) Multi-agent Network Control, (ii) Decision and Neuro Sciences, (iii) Communications and Human Networks, (iv) Intelligent Information Networks, and an International Program, (v) Network Science and Intelligent Systems. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Multi-agent Network Control. The Multi-Agent Network Control program has a long, successful history in providing new scientific results and leadership concerning the mathematical foundations for the robust control of complex real-time physical and information-based systems. The program was among the first in the DoD to recognize the need and potential for mathematical control theory to be pushed toward the heterogeneous multi-agent and (semi)autonomous domain, leading to a strong record of success in the distributed control of autonomous agents as well as the control of micro-biological systems. Concurrent with these developments, the scientific community became keenly aware of the role of interconnections, and dynamics over these interconnections, on the ensuing behavior of finite (oftentimes large) numbers of agents (in the abstract sense). This subsequently led to the burgeoning discipline of "network science" for which principles were sought and discovered and often found a broad range of applications spanning the physical, biological, and social sciences. While discovery and understanding of complex systems in nature, economics, and society are of profound value and impact, our ability to exploit this knowledge to engineer the controllability, fragility, propensity for self-organization, and/or robustness of interdependent dynamical systems will inevitably demonstrate true mastery. Creating the relevant theory to adapt and control science in this regard has emerged as a focal point for future programmatic efforts. An overarching, principled framework has yet to be established and requires not only control theory, but also dynamical systems, information processing, and phenomenological physics. Thus, the mission of the Multi-Agent Network Control program is to establish the physical, mathematical, and information processing foundations for the control of complex networks. In view of complementary ARO Network Science Division efforts spanning intelligent, communication, and sociological networks, the main focus of the program will primarily involve physical and biological networks but in an abstract framework potentially extensible to network models relevant to all division portfolios. This Program Area is divided into three research thrusts: (i) Control and Dynamical Systems Theory, (ii) Information Structure, Causality, and Dynamics, and (iii) Physics in the Control of Complex Networks. These thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal.

2. Social and Cognitive Networks. The goal of the Social and Cognitive Networks program is to develop measures, theories, and models that capture cognitive and behavioral processes that lead to emergent phenomena in teams, organizations, and populations. Social networks allow collective actions in which teams can communicate, collaborate, organize, perform collective tasks, mobilize, or attack. Social influence processes determine how ideological groups form and dissolve, information and beliefs spread and interact, and how populations reach consensus or contested states. Research supported in this program includes both methodological aspects of modeling human networks and substantive work to further our understanding social and emergent phenomena. Methodological projects focus on statistical network analysis, computational models and dynamic simulations that address issues such as scalability, multilayers, and data accuracy (i.e., investigating effects of measurement error on metrics and inferences due to missing, inaccurate or hidden network data). Substantive research focuses on cognitive and psychological factors that drive social phenomena, including development of new metrics, constructs and mechanisms involved with complex activities such as information transfer/exchange and collective decision-making. This program invests in innovative solutions that blend theories and methods from the social sciences with rigorous computational methods from computer science and mathematical modeling. The changing nature of DoD's doctrines and missions have greatly increased the need for models that capture the cognitive and organizational factors that drive activities of groups, teams and populations. The program seeks to advance our understanding of the human dimension and provide critical insights about team coordination and problem solving, social diffusion and propagation, and develop tools that enable inference and modeling of complex social phenomena.

3. Communications and Human Networks. The goal of this Program Area is to better understand the fundamental scientific and mathematical underpinnings of wireless communications and human networking, their similarities, and the interactions between these two networks. This Program Area is divided into two research Thrusts: (i) Wireless Communications Networks and (ii) Human Networks. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research to pursue the program's long-term goal. The Wireless Communications Networks Thrust supports research to discover the fundamental network science principles as they apply to the wireless multi-hop communications systems, while the Human Networks Thrust identifies and supports research to better understand social network structures from heterogeneous data, the structures effect on decision making, and the interaction of communications and human networks. The research efforts promoted by this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications could include wireless tactical communications, improved command decision making, and determining the structure of adversarial human networks.

4. Intelligent Information Networks. The goal of this Program Area is to develop and investigate realizable (i.e., computable) mathematical theories, with attendant analysis of computational complexity, to capture common human activity exhibiting aspects of human intelligence. These studies may provide the foundation for helping augment human decision makers (both commanders and Soldiers) with enhanced-embedded battlefield intelligence that will provide them with the necessary situational awareness, reconnaissance, and decision making tools to decisively defeat any future adversarial threats. This Program Area is divided into two research Thrusts: (i) Integrated Intelligence and (ii) Adversarial Reasoning. These thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long term goal. The Integrated Intelligence Thrust supports research to discover the mathematical structuring principles that allows integration of the sub-components of intelligent behavior (such as vision, knowledge representation, reasoning, and planning) in a synergistic fashion, while the Adversarial Reasoning Thrust area brings together elements of Game Theory, knowledge representation and social sciences to reason about groups/societies in a robust manner. The research efforts promoted by this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications could include robotic unmanned ground and air vehicles, reasoning tools for wild life management, and decision making tools in the context of command, control, communications, computers, intelligence, surveillance and reconnaissance (C4ISR).

5. Network Science and Intelligent Systems (International Program). As one of the ARO International Programs and part of the ARO Network Science Division portfolio, the Network Science and Intelligent Systems program is focused on supporting multi-disciplinary research at institutions outside of the U.S., with the goal to accelerate new discoveries in Network Science. Of particular interest are Wireless Communications and Information Networks, Social Network Analysis and Visualization, Dynamics of multi-genre networks and topics at the intersection of Graph Mining, Machine Learning and Artificial Intelligence.

C. Research Investment

The total funds managed by the ARO Network Science Division for FY17 were $61.1 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY17 ARO Core (BH57) program funding allotment for this Division was $8.0 million and $1.2 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $5.5 million to projects managed by the Division. The Division also managed $43.3 million of Defense Advanced Research Projects Agency (DARPA) programs. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $0.7 million for contracts. In addition, $3.9 million was provided for awards in the Historically Black Colleges and Universities and Minority Serving Institutions (HBCU/MSI) Programs, including funding for DoD-funded Partnership in Research Transition (PIRT), DoD-funded Research and Educational Program (REP) projects, and $1.5 million of the Division's ARO Core (BH57) funds, with the latter included in the BH57 subtotal above.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY17 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY17 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY17, the Division awarded twenty five new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Panos Antsaklis, University of Notre Dame; *Distributed Control of Cooperative Multi-Agent Systems: Combined Top-down and Bottom-up Design*
- Professor Siddhartha Banerjee, Cornell University*; Operations and the Sharing Economy: Mechanisms for On-Demand Resource Sharing with Military Applications*
- Professor Rick Blum, Lehigh University*; Ordering for Hypothesis Testing and Beyond*
- Professor Rene Carmona, Princeton University; *Mean Field Games on Graphs*
- Professor Huaiyu Dai, North Carolina State University; *Understanding and Accelerating Information Spreading in Dynamic Networks*
- Professor Cleotilde Gonzalez, Carnegie Mellon University; *Scaling up models of decisions from experience: Information and incentives in networks*
- Professor Joseph Halpern, Cornell University; *Combining and Abstracting Causal Models*
- Professor Dmitri Krioukov, Northeastern University; *Link prediction and community inference in networks using latent geometry*
- Professor Vikram Krishnamurthy, Cornell University; *Dynamics of Interactive Social Sensors*
- Professor Zongli Lin, University of Virginia; *Coordinated Control of Multi-agent Systems With Real-World Constraints*
- Professor Enrique Garcia Mallada, Johns Hopkins University; *Beyond Consensus: A Distributed Optimization Approach for Complex Coordination in Large-scale Dynamic Networks*
- Professor Natasa Miskov- Zivanov, University of Pittsburgh; *AIM Cancer: Automated Integration of Mechanisms in Cancer*
- Professor Eytan Modiano, Massachusetts Institute of Technology; *Low Latency Wireless Networks for Mission Critical Communications*
- Professor Stephen A Morse, Yale University; *Multi-Agent Estimation and Decision-Making*

- Professor Ashutosh Nayyar, University of Southern California; *Stochastic Dynamic Games of Asymmetric Information: A Common Information Approach*
- Professor Shmuel Oren, University of California – Berkeley; *Computational Methods for Large-scale Interconnected Systems with Continuous and Discrete Parameters*
- Professor Eric Rice, University of Southern California; *Predictive Modeling for Early Identification of Suicidal Thinking in Social Networks*
- Professor Tuomas Sandholm, Carnegie Mellon University; *Steering T-Cell Adaptation Using Opponent Exploitation Algorithms and Computational Game Theory*
- Professor William Sandholm, University of Wisconsin – Madison; *Large Deviations in Multi-Agent Systems*
- Professor Sanjay Shakkottai, University of Texas at Austin; *Leveraging Limited Human Input: An Optimization and Bandits Approach*
- Professor Blair Vida Sullivan, North Carolina State University; *Algorithms for Exploiting Approximate Network Structure*
- Professor Rebecca Willett, University of Wisconsin – Madison; *Inference for High-Dimensional Self-Exciting Point Processes*
- Professor Osman Yagan, Carnegie Mellon University; *Network Science Data-driven Modeling of Information Propagation in Multilayer and Multiplex Networks*
- Professor Jamil Zaki, Stanford University; *Social Network Analysis: Brain predictors of social network structure and function*
- Professor Qing Zhao, Cornell University; *Large-Scale Network Inference: Detecting the Unknown and the Intermittent*

2. Short Term Innovative Research (STIR) Program. In FY17, the Division awarded eleven new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Necdet Aybat, Pennsylvania State University; *Decentralized Methods for Multi-Agent Problems Over Networks*
- Professor Nader Behdad, University of Wisconsin – Madison; *A biologically-inspired, platform-integrated VHF antenna system for compact ground robots*
- Professor Itai Cohen, Cornell University; *Multi-Agent Network Control. Determining the Limits of Human Coordination*
- Professor Gourab Ghoshal, University of Rochester; *Predictability Limits in Human Dynamics as a Function of Data Completeness*
- Professor Sriraam Natarajan, Indiana University at Bloomington; *Human-Machine Collaboration in Relational Sequential Decision-Making Problems*
- Professor Saket Navlakha, Salk Institute for Biological Studies; *Searching for algorithmic principles of adaptive network design and load balancing in the nervous system*
- Professor Dimitra Panagou, University of Michigan - Ann Arbor; *Theory and Algorithms for Safe and Secure Dynamic Multi-Agent Networks*
- Professor Walid Saad, Virginia Polytechnic Institute & State University; *Performance of Wireless Communications using Unmanned Aerial Vehicles*
- Professor Siqian Shen, University of Michigan - Ann Arbor; *Data-driven Risk-aware Adversarial Analysis under Uncertainty*
- Professor Sennur Ulukus, University of Maryland - College Park; *Breaking the square-root barrier in covert communications*
- Professor Tansel Yucelen, University of South Florida; *Multi-Agent Coordination over Prescribed Time Intervals: System-Theoretic Foundations and Distributed Control*
- Professor Justin Zhan, University of Nevada - Las Vegas; *A Deep Learning Framework for Network Dynamics Prediction*

3. Young Investigator Program (YIP). In FY17, the Division awarded four new YIP projects to drive fundamental research in an area relevant to the current and future Army. The following PIs and corresponding organizations were a recipient of the new-start YIP award:

- Professor Raquel Asencio, Purdue University*; Exploring Effective Coordination Structures and Functioning in Multiteam Systems*
- Professor Fabio Pasqualetti, University of California – Riverside*; Design and Operation of Secure Multi-Agent Networks*
- Professor Tyler Summers, University of Texas at Dallas; *Quantifying network controllability and observability using optimal control and estimation metrics*
- Professor Timothy Weninger, University of Notre Dame; *Mining Conversation Trails for Effective Group Behavior*

4. Conferences, Workshops, and Symposia Support Program. The Division provided funds in support of a range of scientific conferences, workshops, and symposia that were held in FY17. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences, with the goal of supporting scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army, and to define the research needs, thrusts, opportunities, and innovation crucial to the future Army. Proposals requesting funding support, typically for less than $10K, were received and evaluated in line with the publicly available ARO BAA. In FY17, seven proposals were selected for funding by the Division to support FY17 conferences, workshops, or symposia.

5. Special Programs. In FY17, the Division also awarded four new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school and undergraduate students. These efforts were funded through the ARO Core Program and Youth Sciences Programs, for research to be performed at academic laboratories currently supported through active SI awards (refer to CHAPTER 2, Section IX).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Network Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Scalable, Stochastic and Spatiotemporal Game Theory for Adversarial Behavior. This MURI began in FY11 and was awarded to a team led by Professor Milind Tambe of the University of Southern California, with participation from researchers at UCLA, Duke University, Stanford University, UC Irvine and California State University at Northridge. The objective of this MURI is the development of game theory formalisms that account for bounded rationality, scalability of solutions, real-world adversaries, and socio-temporal issues. The technical approach to be followed by the team will involve a mix of behavioral experiments and development of theoretical formalisms to characterize individual human behavior and that of adversarial groups; it is expected that psychological theories such as prospect theory and stochastic theories for coalitional games will play equal part in the technical development. The results of this MURI may have significant impact on diverse applications of the Army such as the monitoring of contracts while building nations or societies.

2. Evolution of Cultural Norms and Dynamics of Socio-Political Change. This MURI began in FY12 and was awarded to a team led by Professor Ali Jadbabaie of the University of Pennsylvania, with participation from researchers at MIT, Stanford, Cornell, and Georgia Tech. The objective of this MURI is to find synergy in methods and models from work in social sciences, engineering, network sciences, and mathematics to develop new techniques and mathematical models that would explain societal events not *posterior* but as they are happening, based on detailed analytical models of social systems. The team hopes to use a unified yet interdisciplinary lens that goes beyond social and political sciences, and adequately covers the full spectrum from rigorous math-based theory and modeling to large scale data extraction and analyses and from multi-agent simulation to controlled lab experiments and field surveys. The results of the MURI may have significant impact on the Army and DoD to understand cataclysmic changes, such as the Arab Spring, as they are about to happen.

3. Control of Complex Networks. This MURI began in FY13 and was awarded to a team led by Professor Raissa D'Souza of the University of California at Davis. The goal of this MURI project is to develop rigorous principles to predict and control behaviors of systems made of interdependent networks. This will be accomplished through an interdisciplinary approach synthesizing mathematical theories from statistical physics, control theory, nonlinear dynamics, game theory, information theory, system reliability theory, and operations research. The results will be informed and validated by empirical studies of real-world systems from nanoscale mechanical oscillators, to collections of interdependent critical infrastructure systems, to data on coalitions and conflict in primate societies, to longitudinal data on the evolution of political networks of nation states and task-oriented social networks in open source software. The focus is to develop new approaches that exploit network interdependence for network control, and this diversity of empirical testbeds is central to developing robust theoretical principles and widely applicable methods.

It is expected that this MURI will lead to (i) network interventions that prevent cascades of failure in critical infrastructures, (ii) novel control schemes relying on control actions and local interventions, (iii) rigorous principles for multi-modal recovery of heterogeneous systems, (iv) shaping human social response via designed incentives that align human behavior with the capabilities of technological networks, (v) design of networks of nonlinear nanoelectromechanical oscillators that exploit coupling and nonlinearity to create coherent motion, (vi) new mathematical structures for representing and analyzing networks-of-networks, especially with respect to control theory, and (vii) fundamental bounds on controllability of interdependent networks and rigorous techniques to identify which network layers are easiest to steer.

The anticipated impact on DoD Capabilities is broadly applicable to controlling a disparate collection of autonomous agents interacting through numerous networks in noisy, dynamic environments with a myriad of time-scales and length-scales. Results can be applied to security (and restoration) of critical infrastructures, supply chains, political alliance dynamics (including upheavals such as Arab Spring), conflict, risk, social dynamics, and collective action. It is also reasonable to expect that there will be new levels of nanoscale functionality in the NEMs device developed, enabling new technologies and devices.

4. Network Science of Teams. This MURI began in FY15 and was awarded to Professor Ambuj Singh of the University of California at Santa Barbara, with participation from researchers at University of Southern California, University of Illinois at Urbana-Champaign, Northwestern University, and MIT. These seven faculty provide an excellent balance of multidisciplinary scholars from sociology, cognitive and social psychology, health and behavioral sciences, computer science, statistics, controls and dynamical systems, and network science. This MURI will advance the development of the Network Science of Teams by creating quantitative, network-based models of adaptive team behavior. This research will produce methods to optimize team performance under different contexts and resource constraints. The three thrusts of this research effort include (i) teams as networks of interacting entities, (ii) analysis and models of dynamic team behavior over task sequences, and (iii) the network science of teams-of-teams or multi-team systems. The overarching objectives of this research are to build quantifiable informative models of team behavior as dynamical systems interacting over multiple networks, to develop rigorous models that relate interaction patterns and network evolution to task performance, to break new ground in the learning of optimal design of teams for complex tasks, and to advance social science theories of team performance. This MURI will have a significant impact for the Army and DoD with respect to how it conducts its work in teams in that results from this research may help the Army and joint forces assemble more effective teams and teams of teams, and provide guidance on task sequencing to support their highest goals.

5. Multi-modal Analytics to Understand Latent Communication. This MURI began in FY16 and was awarded to a team led by Professor V. S. Subrahmanian of the University of Maryland. The goal of this MURI is two fold: (i) develop social science theories to understand latent communication among a small group of adversaries engaged in an effort to deceive, and (ii) develop multi-media analytics tools that formalize those social science theories as algorithms which can aid an observer who is not steeped in the local culture. While driven by practical problems, the objectives of the proposed work is not only to drive the development of new social science theories, but also to drive algorithmic advances in reasoning about joint probability distributions that arise from modeling uncertainties in human actions, speech, gestures, and intentions.

C. Small Business Innovation Research (SBIR) – New Starts

Research within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY17, the Division managed one new-start SBIR contract, in addition to active projects continuing from prior years. The new-start projects consisted of one Phase II contract. This new-start contract aims to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY17 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY17, the Division managed one new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of one Phase II contract. This new-start contract aims to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY17 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Serving Institutions (HBCU/MSI) – New Starts

The HBCU/MSI program encompasses the (i) Partnership in Research Transition (PIRT) Program awards, (ii) DoD Research and Educational Program (REP) awards for HBCU/MSIs, and (iii) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY17, the Division managed one new REP award, in addition to active projects continuing from prior years. In addition, proposals from HBCU/MSIs are often among the projects selected for funding by the Division (refer to the list of HBCU/MSI new starts in *CHAPTER 2, Section IX*.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

No new starts were initiated in FY17.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY17, the Division managed four new DURIP projects, totaling $1.05 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. DARPA Big Mechanism Program

The Big Mechanism program attempts to understand conflicting information available in research literature on any big mechanism. The chosen area for the program is Cancer Biology, while the resulting techniques could be applied to a number of other mechanisms including climate change, with each piece of published work contributing a small portion of understanding to the big mechanism. The effort should lead to advances in the Natural Language Processing for automatically extracting information for scientific literature, advances in knowledge representation for signaling pathways with potential ambiguities in cancer biology, resolution of information from new publication against what is already known, and potential for advancement in explanation of causality of how cancer cells grow. This program is managed on behalf of DARPA through the Network Science Division, Intelligent Networks Program.

I. DARPA SIGMA Program

The SIGMA program is an effort to understand the issues associated with deploying a large sensor network for detection of nuclear threats in an urban environment. The concept of the program is to develop a very large network of sensors, that can be carried by people, but require no interaction. The program includes development of the sensors, communication networking via smart phone devices, and processing and fusing very large amounts of data. Communications and networking issues include security and privacy as well as dealing with data transfer from a large number of sensors. Portions of this program dealing with the sensor communications and networking as well as research into human factors dealing with technology adoption are managed on behalf of DARPA through the Network Sciences Division, Communications and Human Networks Program.

J. DARPA Communicating with Computers (CwC) Program

The goals of the DARPA Communicating with Computers program are to advance the state of the art in text and video analytics to the extent that a machine and its human operator can have the same mental model. This requires that the machine be able to understand the human intent, and that it can explain back, to the human, in ways that makes use of the context and prior knowledge. Three challenge problems have been chosen: (i) playing a game of blocks between humans and machines, (ii) a bicuration assistant that helps a human investigate knowledge representation of signaling pathways in cancer biology, and (iii) an author's assistant that could help a human write stories. This program is managed on behalf of DARPA through the Network Science Division, Intelligent Networks Program.

K. DARPA Computational Simulation of Online Social Behavior (SocialSim) Program

The goal of the DARPA Computational Simulation of Online Social Behavior (SocialSim) program is to develop innovative technologies for high-fidelity computational simulation of online social behavior focused on the spread and evolution of online information while rigorously testing and measuring simulation accuracy. The SocialSim program is centered around three objectives: (i) develop technologies that can accurately simulate online information spread and evolution at scales representing populations of interest (i.e., thousands to tens of millions); (ii) develop efficient and robust methods for providing data to support simulation development, testing, and measurement; and (iii) develop rigorous methods and metrics for quantitatively assessing the accuracy and scalability of simulations of online information spread and evolution. This program is managed on behalf of DARPA through the Network Science Division, Social and Cognitive Networks Program.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Network Sciences Division.

A. Quantifying Cognitive Factors in Online Social Behavior

Professor Kristina Lerman, University of Southern California, Single Investigator Award

The objective of this research is to measure the impact of cognitive factors on individual choices and the collective outcomes of those choices. In FY17, Professor Kristina Lerman at the University of Southern California's Information Sciences Institute focused her research on understanding the ways people make decisions to allocate attention and the role that cognitive factors play in these decisions. Of specific focus was the biases important in online interactions, such as message position bias, social influence bias, and affect biases. Professor Lerman and her team tested and validated hypotheses with empirical data from a variety of sources including Stack Exchange (an online Question and Answer forum), reddit (a social media platform for collectively sharing and rating news stories), and experimentally collected data.

In FY17, the team analyzed data from 250 communities on the Stack Exchange network to pinpoint factors affecting which answers are chosen as the best answers. Through empirical analysis of human behavioral data and using penalized logistic regression, the research team identified features associated with users' individual decisions in a crowdsourcing question and answer expertise system. They discovered that cognitive bias (heuristics or mental shortcuts) and cognitive load (amount of information an individual is processing at once) can degrade collective wisdom of crowds. The largest regression coefficients were associated with features related to answer salience (web page order and word share per answer), suggesting that rather than evaluate all available answers, users rely on cognitive heuristics to select the perceived best answer especially when the cognitive load (as measured through the number of answers to choose from) increased (see FIGURE 1). To test the impact of this effect, the researchers conducted a controlled human subjects experiment using a choice set of two compared to eight answers: when two answers were shown, workers were about 50% more likely to pick the answer at the top of the screen, but when eight answers were shown, they were twice as likely to do so.

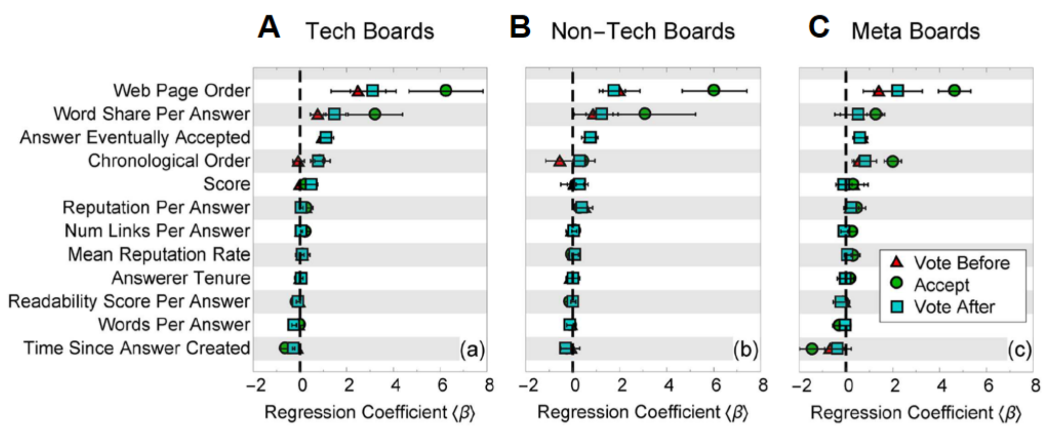

FIGURE 1

Relative size of regression parameters for answer acceptance and voting. Regression coefficients for answerers to accept (circles) and voters to vote for an answer before (triangles) and after (squares) an answer is accepted on (**A**) technical, (**B**) non-technical, and (**C**) meta boards, averaged over the number of available answers from two to twenty. Higher values indicate a stronger relationship between attributes and user behavior (voting or accepting an answer). Error bars indicate the variance of the best-fit values across two to twenty answers. [1]

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[1] Burghardt K, Alsina EF, Girvan M, Rand W, Lerman K (2017) The myopia of crowds: Cognitive load and collective evaluation of answers on Stack Exchange. *PLoS ONE* 12: e0173610.

Collectively, these results provide strong evidence that, rather than evaluate all available answers to a question, users rely on simple cognitive heuristics to choose an answer to vote for or accept. These cognitive heuristics are linked to an answer's salience, such as the order in which it is listed and how much screen space it occupies. While askers appear to depend on heuristics to a greater extent than voters when choosing an answer to accept as the most helpful one, voters use acceptance itself as a heuristic, and they are more likely to choose the answer after it has been accepted.

B. Coding for Networks with Adversaries

Professor Aaron Wagner, Cornell University, Single Investigator Award

The objective of this research is to design resilient communication systems (i.e., communication systems that provide reasonable performance guarantees even in the face of adversarial attacks). It focuses on the Man-In-The-Middle (MITM) attacks, in which an adversary is assumed to successfully have injected himself in a network somewhere between the transmitter and the receiver. The adversary then seeks to disrupt the communication as much as possible by altering portions of the transmission while it is en route, which could take the form of physical-layer jamming or altering, deleting, or inserting packets at higher layers in the stack (see FIGURE 2). This form of resilience is particularly relevant to military systems, and system that are resilient against MITM attacks will generally be resilient against other, more benign, disruptions as well.

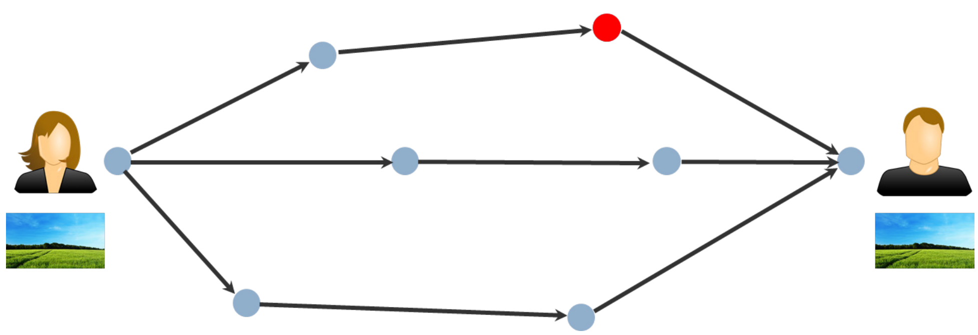

FIGURE 2

Multi-hop multipath communications with adversary, denoted in red.

While conventional cryptographic methods and error correcting codes can be used to detect that the adversary has altered some packets in a stream and to correct these errors if they are very few, they suffer from an "all-or-nothing" behavior: unless the receiver can recover all of the transmitted data, it cannot recover any of it. Thus a stream must be completely discarded unless it is possible correctly identify all of the changes the adversary made to the stream. This allows an adversary to render large amounts of traffic unusable by altering just enough to make full recovery impossible. The goal of this work is to design networks that allow receivers to identify and extract portions of a data stream that are provably unaltered by the adversary, even if the adversary has altered enough packets to make it impossible to recover all of the data. Armed with such protocols, the network designer can assure that adversaries that alter a small amount of traffic can cause only small---ideally negligible---disruptions in the operation of the network.

In FY17, Professor Wagner developed a unique coding strategy for the case when multiple paths exist to transmit a data file, but the adversary only has access to one or a few paths. This code allows the receiver to completely reconstruct the data when there is no adversary and reconstruct portions of the data when the adversary attacks a portion of the paths. The code is unorthodox in that it relies on arithmetic operations over the real numbers. Virtually all conventional error-correcting codes are uses finite-field operations instead. This distinction is crucial because our code is able to beat conventional schemes by relying on properties of Euclidean geometry that do not have finite-field analogs. The novelty of this approach suggests that it might have other applications, and its use in other domains, such as distributed storage are currently being investigated. There are results that show when it is feasible to use these codes and optimality results that justify the code design and show that the resulting decoder is optimal.

C. Quantifying network controllability and observability using optimal control and estimation metrics

Professor Tyler Summers, University of Texas at Dallas, Single Investigator Award

Since 2011 there has been increasing interest in characterizing the number of nodes needed to ensure structural controllability in a network of dynamical systems. It has been argued that control over a small subset of nodes is all that is needed to ensure controllability of a complex network of dynamical systems. Different perspectives on network controllability have been recently used to provide a rigorous characterization of the fundamental limits of control in complex networks. In particular, these issues have been examined in the context of sensor selection and Kalman filtering in a network.

In FY17, the PI contributed to this endeavor by deriving a set of performance bounds for dynamical networks in terms of optimal feedback control performance. The bounds characterize a tradeoff between achievable feedback control performance and the actuator structure. For example, when the network dynamics are unstable, the optimal cost can increase exponentially with the size of the network for any fixed-size actuator set. The implication of this is that feedback control costs may be extremely high even with an optimal selection of a fixed number of actuators.

D. Steering T-Cell Adaptation Using Opponent Exploitation Algorithms

Professor Tuomas Sandholm, Carnegie Mellon University, Single Investigator Award

Working with biologist at Carnegie Mellon University, an objective of this research is to develop a novel rule-based model of the T cell differentiation pathway that is based on a Boolean model, but also considering concentrations of signaling elements and reaction rates that cannot easily be incorporated in the Boolean framework. Thus, rule-based simulations results reflect realistic time scales of protein interactions and enzyme kinetics, in addition to changes in protein and mRNA abundance, that allow tight integration between model predictions and experimental data. In addition to protein interactions, transcription, and translation, the rule based model of T cell differentiation explicitly defines post-translational modifications central to the receptor activated signaling pathways. One of the key aspects of this hybrid model is the ability to model shared IL2 pool, as this allows to model a whole population of cells, each contending part of the common pool. This type of inter-cell communication was not possible in the Boolean model. In FY17, Professor Sandholm also wrote an automatic system that can take any rule-based model and convert it into an efficient numerical simulator, which has been helpful in communicating with the biologists. Finally, all of this work has led to Stackelberg games with limited look-ahead capturing partial knowledge, and bounded rational agents (such as biological agents).

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Unified Approach to Abductive Inference Investigator:

Professor Pedro Domnigos (lead PI), University of Washington, and Professor Carlos Guestrin (co-PI), University of Washington, MURI Award
Recipient: Apple, Inc.

The goals of the MURI was the development of a framework to reason about potential causes for a set of observations. In order to create this framework, it was necessary to generate schemes for very efficient belief propagation algorithms. During the MURI, Professor Guestrin and his students created a framework called GraphLab, which was then used within the project for test theories on abductive reasoning. Realizing the commercial potential of the toolset, Professor Guestrin launched a company called GraphLab. The company was later renamed Turi, and subsequently, was sold to Apple Inc. for over $200M during the last quarter of 2016. Turi, situated in Seattle, WA, now serves as the AI Research Lab for Apple, Inc.

B. Spatio-Temporal Game Theory

Investigator: Professor Milind Tambe, University of Southern California, MURI Award
Recipient: Sherrif's Office, City of Los Angeles, CA

The goal of this MURI is the development of a framework for modeling boundedly-rational actors in 2-person games, and in particular, with respect to security games. Furthermore, the work of Professor Tambe's team proposed to consider multi-shot games and the effect of taking into account resources, space, people, and other factors. One particular strand of work on Stackelberg Games (a particular kind of security game) has recently been deployed by the LA Sheriff's department for patrolling trains in Los Angeles Metro, where buying tickets is based on an honor system, and as a result is rife for cheating and exploitation. Based on baseline information, and survey of the number of people using the Metro system, cheating has been reduced by over 50%.

C. Spatio-Temporal Game Theory

Investigator: Professor Jeff Brantingham, University of California - Los Angeles, MURI Award
Recipient: Predictive Policing Co.

The goal of this MURI is to development a framework for modeling boundedly-rational actors in 2-person games, with particular interest in security games. Furthermore, the work of Professor Tambe led the team of researchers to consider multi-shot games and the effect of taking into account resources, space, people, and other important variables when necessary.

Using game theoretic ideas, this particular strand of work led to the development of crime prediction tools, including software. Dr. Brantingham, who is the task leader for this goal, started a new company called Predictive Policing. The company sells crime prediction software and services to police departments across the county, which has among its clients, the L.A. Police Department.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Understanding and Accelerating Information Spreading in Dynamic Networks

Professor Huaiyu Dai, North Carolina State University, Single Investigator Award

In many existing and emerging large-scale networks, an important application is to spread the information quickly and efficiently over the network. This topic has received great research interest, and is relatively well studied for static networks. In contrast, when the network structures change over time, information spread is not well understood, which is typical for many applications and particularly true for military operations. Professor Dai's proposed research will advance this understanding and improve algorithm designs for efficient information spreading in various large-scale dynamic networks. This research is divided into two interrelated thrusts, dealing with wireless communication networks and social networks. The first research thrust is devoted to better understanding of information spreading in dynamic networks. Building on promising preliminary results, a unifying analytical framework for mobile networks will be investigated can address various types of mobility patterns and handle both connected and sparse scenarios. The second thrust will utilize and extend the framework to investigate social networks and multilayer networks, which possess unique features and extra resources for information spreading that deserve separate and in-depth considerations. As emerging large-scale networks are complex and exhibit unpredictable dynamics, random walk based algorithms become an appealing architectural solution for them. If successful, this research will contribute a general analytical framework that can further our understanding of information spreading in dynamic complex networks, and provide insights for design and optimization of practical algorithms and protocols that directly address the Army's needs for multi-dimensional network-centric operations.

B. Towards Optimal Teams in Composite Networks

Professor Hanghang Tong, Arizona State University, Single Investigator Award

Professor Hanghang Tong seeks to develop new algorithms to (re)design teams to better configure and utilize limited human resources for improved performance gains. It is anticipated that in FY18, this research will explore the utilization and exploitation of composite networks comprised of social networks, information networks, and cognitive networks to identify dimensions for optimization of collaborative human performance. Of specific focus will be exploring the ways to bring key network metrics that drive peak team performance into the team search, formation, and refinement process. Further, this work will focus on developing ways to help organizational decision-makers make a better decision to perform certain tasks that need collaborative effort within a team through improved configuration of limited network and human resource.

Professor Tong will approach this problem with a multi-disciplinary perspective, consisting of network query, visualization, and optimization. In FY18 it is anticipated that the research team will develop a formulization for team search as a complex network browsing and query problem, where the researchers seek to build interactive, user-friendly, and scalable systems to search for desired teams. The team will formulate the team formation problem as a multi-team, multi-objective, and multi-level optimization problem whose objective function integrates different key network metrics that drive the peak team performance with a careful balance between different metrics that quantifies both the skill matching and the structural matching of potential team members. If successful, this research will lead to the development of software tools that can be utilized to optimize team performance, in situations of limited resources, on both the task and human dimensions.

C. Time-varying Actuation and Interconnection in Network Systems

Professor Jorge Cortes, University of California (UC) - San Diego and Prof. Fabio Pasqualetti UC – Riverside, Single Investigator Award

Network structure plays a critical role in shaping properties of interconnected dynamical systems. This is particularly relevant in the human brain, as the empirical evidence suggest that the organization of neural circuits determines healthy vs. diseased functions, regulates information processing, and affects cognitive performance. To objective of this research is to (i) analyze time-varying synchronization patterns in brain networks with new theories and tools aimed at characterizing how localized perturbations may have their network-wide effects and (ii) study optimal information transmission (and possibly control) of brain networks by exploiting the geometric structure of interconnection patterns for well-defined cognitive processing tasks.

In FY18, it is anticipated the investigators will be able to characterize how localized perturbations may have network-wide effects through the utilization of their analysis of time-varying synchronization patterns in brain networks and theoretical tools from network control. The investigators will also study optimal information transmission (and possibly control) of brain networks by exploiting the geometric structure of interconnection patterns for well-defined cognitive processing tasks.

D. Understanding Social Influence without Markov Assumptions

Professor Paulo Shakarian, Arizona State University, Single Investigator Award

There have been numerous empirical studies that have explored many facets of peer-based social influence in online communities - and these have included studies that ranged from social simulations to controlled experiments to large-scale studies on social media sites. A separate line of research on social cascades has also been explored. In these studies, a progression of influence events leads to ideas spreading in large populations on the Internet. The study of these macro-characteristics of cascades is currently a very active area of research. However, it is important to realize that cascades are built on peer-based influence activities and in such cases peer-based influence occurs in the context of these cascades. Further, in viewing influence in the context of a cascade, many assumptions of current modeling techniques become questionable - perhaps most strikingly is the Markovian assumption that assumes that a given peer-influence action is independent of all previous interactions. This leads us to two very important open questions: i) how does peer influence change in the context of a spreading cascade and ii) can we develop models to characterize peer influence in this context. This inherently is problematic as the knowledge of a vastly spreading cascade may itself be a factor in peer influence. To address these questions, in FY18 it is anticipated that Professor Shakarian and his colleagues will develop an inductive rule learning framework that allows for the automatic generation of transparent models of influence that do not rely on the Markovian property. Furthermore, Professor Shakarian is also conducting empirical studies to generate data that can be analyzed with their non-Markovian framework.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Purush Iyer
Division Chief
Program Manager, Intelligent Networks

Dr. Alfredo Garcia
Program Manager, Multi-Agent Network Control

Dr. Edward Palazzolo
Program Manager, Social and Cognitive Networks

Dr. Robert Ulman
Program Manager, Communication and Human Networks
Program Manager, Network Science and Intelligent Systems (International)

B. Directorate Scientists

Dr. Randy Zachery
Director, Information Sciences Directorate

Dr. Bruce West
Senior Scientist, Information Sciences Directorate

Ms. Anna Mandulak
Contract Support

C. Administrative Staff

Ms. Debra Brown
Directorate Secretary

Ms. Diana Pescod
Administrative Support Assistant

CHAPTER 11: PHYSICS DIVISION

I. OVERVIEW

As described in *CHAPTER 1*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2017* is to provide an annual historical record summarizing the programs and basic research supported by ARO in FY17. ARO's mission is to support creative basic research resulting in new science that enables new materials, devices, processes, and capabilities for the current and future Soldier. This chapter provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions enabled by the ARO Physics Division in FY17.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Physics Division supports research to discover exotic quantum and extreme optical physics. The Division promotes basic research that explores frontiers where new regimes of physics promise unique function. Examples such as ultracold molecules, topological physics, attosecond light pulses, and quantum entanglement all represent areas where the scientific community's knowledge must be expanded to enable an understanding of the governing phenomena. The results of this research will stimulate future studies and help to keep the U.S. at the forefront of research in physics.

2. Potential Applications. Research managed by the Physics Division will provide a scientific foundation upon which revolutionary future warfighter capabilities can be developed. The Division's research is focused on studies at energy levels suitable for the dismounted Soldier: the electron Volt and milli-electron Volt range. In the long term, the discoveries are anticipated to impact warfighter capabilities in the area of Command, Control, Communications, Computers, Intelligence, Surveillance, and Reconnaissance (C4ISR). Research advances in the Division can be readily visualized to impact sensor capabilities for increased battlespace awareness and Soldier protection, enhanced navigation, ultra-lightweight optical elements and energy-efficient electronics for decreased Soldier load, increased Soldier awareness, and advanced computational capabilities for resource optimization and maximal logistical support.

3. Coordination with Other Divisions and Agencies. To meet the Division's scientific objectives and maximize the impact of discoveries, the Physics Division coordinates and leverages research within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), and the Defense Advanced Research Projects Agency (DARPA). In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multidisciplinary research topics, and evaluate the effectiveness of research approaches. For example, research co-funded with the Mathematical Sciences Division seeks coherent-feedback quantum control of collective hyperfine spin dynamics in cold atoms. The Division coordinates its research portfolio with AFOSR and DARPA in pursuit of forefront research involving ultracold molecules and optical lattices. The Division also coordinates certain projects with Intelligence Advanced Research Projects Activity (IARPA) and other government agencies. These interactions promote a synergy among ARL and DoD agencies, and improve the quality of the Division's research areas.

The Division's research portfolio will also reveal previously unexplored avenues for new Army capabilities while also providing results to support the ARL ERAs of (i) Impact of Operating in a Contested Environment, and (ii) Implementation. In addition, the Division supports the (i) the Materials Research Campaign's goals to determine how quantum processes could be harnessed for quantum memory and secure communication, and to explore and exploit recent advances in interface physics between unique materials, (ii) the Information Sciences Campaign's goal to explore techniques, architectures, and properties that take advantage of the quantum and related effects for transmitting information, and (iii) the Sciences for Lethality-and-Protection Campaign's goal to identify, exploit, and protect against the effects of directed and non-directed application of energy.

B. Program Areas

The Physics Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY17, the Division managed research within these five Program Areas: (i) Atomic and Molecular Physics, (ii) Condensed Matter Physics, (iii) Optical Physics and Fields, (iv) Quantum Information Science, and an International Program, (v) Quantum Scale Materials. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have long-term goals that support the Division's overall objectives.

1. Atomic and Molecular Physics. The goal of this Program Area is to study the quantum properties of atoms and molecules and advance a fundamental understanding of exotic quantum behavior. When a gas of atoms is sufficiently cooled, the quantum nature dominates and the atoms behave wave-like rather than a cloud of distinct particles. Accordingly, experiments that were once the sole purview of optics are now possible with matter: interference, lasing, diffraction and up/down-conversion, to name a few. This Program Area explores these concepts with an eye toward enabling new opportunities, such as novel quantum chemistry and atomic devices that exploit quantum behavior. The specific research Thrusts within this Program Area are: (i) State-dependent Quantum Chemistry, (ii) Atomtronics, and (iii) Non-equilibrium Many-body Dynamics. Ultracold gases can be trapped in 1D, 2D, or 3D standing optical waves enabling the exploration of novel physics, quantum phase transitions, and mechanisms operative in condensed matter. In optical lattices, one can also create a new "electronics", called atomtronics, based on atoms and molecules having statistics, mass, charge, and many additional handles not available in conventional electronics. The program is not focused on synthesis but rather on the underlying *mechanisms*, such as electronic transport, magnetic response, coherence properties (or their use in molecule formation/selection), and/or linear and nonlinear optical properties. While the notion of taking objects held at sub-Kelvin temperatures onto a battlefield may seem irrational, dilute atomic gases can be cooled to nano-Kelvin temperatures without cryogens by using magnetic traps and lasers. The long-term applications of this research include ultra-sensitive detectors, time and frequency standards, atom lasers and holography, along with breakthroughs in understanding strongly-correlated materials and to design them from first principles.

2. Condensed Matter Physics. The objective of this Program Area is to discover and characterize novel quantum phases of matter in topologically non-trivial matter and in non-equilibrium settings. Topological matter represent a relatively recent discovery of a state of matter defined by the topology of the material's electronic band structure rather than a spontaneously broken symmetry. What is unique about this particular state is that unlike the quantum Hall state, which is also characterized by a topology as it can exist at ambient conditions: room temperature and zero magnetic field. While topological effects have not been observed at these conditions, efforts continue to reach this regime. Furthermore, a host of unique topological states have been discovered, each expressing unique physical phenomena. Unique non-equilibrium phenomena are also being discovered in solid state systems enabled by advanced theoretical and experimental tools as well as novel materials. The majority of these discoveries involve ultrafast infrared or THz radiation impinging on materials that exist near phase transitions in the ground state. In general, discovering and experimentally demonstrating novel phases of matter, both topological and non-equilibrium, will lay a foundation for new technological paradigms. A critical component for gaining new insights is the development of unique instrumentation, therefore construction and demonstration of new methods for probing and *controlling* unique quantum phenomena are also supported.

3. Optical Physics and Fields. The goal of this Program Area is to explore the formation of light in extreme conditions and the novel manipulation of light. Research is focused on physical regimes where the operational physics deviates dramatically from what is known. The specific research thrusts within this Program Area are Extreme Light and Meta-optics. In addition, any fundamental fields that carry energy and information are of interest. The Extreme Light thrust involves investigations of ultra-high intensity light, light filamentation, and femtosecond/attosecond laser physics. High-energy ultrashort pulsed lasers have achieved intensities of 10^{22} W/cm^2. Theoretical and experimental research is needed to describe and understand how matter behaves under these conditions, including radiation reaction and spin effects, from single particle motion to the effects in materials, and how to generate these pulses and use them effectively. One consequence of ultra-high power lasers is light filamentation, which creates a supercontinuum of coherent light across the visible spectrum. Ultra-short intense pulses can be utilized to develop attosecond pulses by combining them with high harmonic generation. Potential long-term applications include imaging through opaque materials, laser pulse modulation, "observing" electron dynamics, and even controlling electron dynamics. Research in the Meta-optics thrust includes studies of optical angular momentum (OAM) beams, interactions with metamaterials, and novel optical physics. An example is the study of OAM beams and how they interact with metamaterials, or how they can be used to induce new kinds of interactions or physics. Another area of interest regards overcoming losses in metamaterials. Cloaking is a well-known idea, but losses and the dispersion must be overcome before this is a reality in the practical sense. In addition, other fields which may be used in place of electrodynamics are of interest to this program. Examination of parity-time symmetric optics is being considered to understand and compensate for loss; topological photonics, Chern number calculation, and topological interactions are also of interest. More generally, research in supersymmetric optics and its relation to topological effects are of interest.

4. Quantum Information Science. The objective of this Program Area is to understand, control, and exploit nonclassical, quantum phenomena for revolutionary advances in computation, sensing, and secure communications. Three major Thrusts are established within this program: (i) Foundational Studies, (ii) Quantum Computation and Networking, and (iii) Quantum Sensing and Metrology. Research in the Foundational Studies Thrust involves experimental investigations of the wave nature of matter, including coherence properties, decoherence mechanisms and mitigation, entanglement, nondestructive measurement, complex quantum state manipulation, and quantum feedback. The objective is to ascertain current limits in creating, controlling, and utilizing information encoded in quantum systems in the presence of noise. Of particular interest is the demonstration of the ability to manipulate quantum coherent states on time scales much faster than the decoherence time, especially in systems where scalability to many quantum bits and quantum operations is promising. Quantum Computation and Networking entails experimental demonstrations of quantum logic performed on several quantum bits operating simultaneously. Demonstrations of quantum feedback and error correction for multiple quantum bit systems are also of interest. There is particular interest in developing quantum algorithms for solving NP-complete problems for use in resource optimization and in developing quantum algorithms to simulate complex physical systems. Research in the Quantum Sensing and Metrology Thrust involves studying the transmission of information through quantum entanglement, distributed between spatially separated quantum entities. Long-range quantum entanglement, entanglement transfer among different quantum systems, and long-term quantum memory are of interest. An emerging field of interest is quantum sensing and metrology using small entangled systems. Entanglement provides a means of exceeding classical limits in sensing and metrology and the goal is to demonstrate this experimentally.

5. Quantum Scale Materials (International Program). As one of the ARO International Programs and part of the ARO Physics Division portfolio, the Quantum Scale Materials Program Area is focused on supporting multidisciplinary research at institutions outside of the U.S., with the goal to accelerate new discoveries in quantum scale materials. Specific research topics of interest include topological states of matter and photons, matter and photons that can support anyon quasiparticles, quantum phase transitions, non-equilibrium quantum dynamics, materials for quantum information processing, quantum metrology with atoms, ions and photons, quantum networks, quantum sensors, and quantum information effects, such as effect of measurement independence on quantum algorithms, such as teleportation, quantum communication and quantum computing.

C. Research Investment

The total funds managed by the ARO Physics Division for FY17 were $145.0 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY17 ARO Core (BH57) program funding allotment for this Division was $8.7 million and $1.9 million of Congressional funds (T14). The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $8.1 million to projects managed by the Division. The Division also managed $16.0 million of Defense Advanced Research Projects Agency (DARPA) programs, and $108.3 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $0.4 million for contracts. In addition, $1.8 million was provided for awards in the Historically Black Colleges and Universities and Minority Serving Institutions (HBCU/MSI) Programs, including funding for DoD-funded Partnership in Research Transition (PIRT), DoD-funded Research and Educational Program (REP) projects, and $0.2 million of the Division's ARO Core (BH57) funds, with the latter included in the BH57 subtotal above.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY17 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY17 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY17, the Division awarded 16 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Warwick Bowen, The University of Queensland (Australia); *Nonequilibrium quantum dynamics in superfluid helium;*
- Professor Kenneth Brown, Georgia Tech Research Corporation; *Control and Spectroscopy of Single Molecular Ions*
- Professor Kyeongjae Cho, University of Texas - Dallas; *Ab Initio Study on Graphene Edge/Super Conductor Contact Interfaces*
- Professor Demetrios Christodoulides, University of Central Florida; *Supersymmetry in Optics & Photonics*
- Professor Jonathan Dowling, Louisiana State University and A&M College; *From Quantum Computation to Quantum Sensing, Imaging, and Metrology*
- Professor Alexander Gaeta, Columbia University; *Development of Chip-Based Optical Parametric Oscillators for Coherent Computing and Quantum Random Number Generation*
- Professor Kenan Gundogdu, North Carolina State University; *Investigation of Room Temperature Electron-Hole Liquid in Atomically Thin Semiconductors*
- Professor Aram Harrow, Massachusetts Institute of Technology (MIT); *New Frameworks for Quantum Algorithms*
- Professor Min-Hsiu Hsieh, University of Technology Sydney (Australia); *Benchmarking Quantum Communication Systems: An Error Exponent Approach*
- Professor Stephen Jordan, University of Maryland - College Park; *Complexity-theoretic Foundations for Near-term Quantum Computers*
- Professor Junichiro Kono, William Marsh Rice University; *Optical Probes and Electron Correlations in Far-From-Equilibrium Graphene*
- Professor Natalia Litchinitser, State University of New York (SUNY) - Buffalo; *Supersymmetry in linear and nonlinear optics*

- Professor Gennady Shvets, Cornell University; *Investigations of Photonic Topological Structures Based on Metallic and All-Dielectric Metamaterials*
- Professor James Williams, University of Maryland - College Park; *Investigations of Candidate Topological Crystalline Insulator SnTe and Pb(1-x)Sn(x)Te*
- Professor Amir Yacoby, Harvard University; *Quantum Sensing of Quantum Materials*
- Professor Chuanwei Zhang, University of Texas - Dallas; *Quantum Phases and Dynamics of Periodically Driven Ultra-Cold Atomic Gases*

2. Short Term Innovative Research (STIR) Program. In FY17, the Division awarded one new STIR project to explore high-risk, initial proof-of-concept ideas. The following PI and corresponding organization was the recipients of the new-start STIR award.

- Professor Jianing Han, University of South Alabama; *Creating and controlling THz superradiance in an ultracold gas*

3. Young Investigator Program (YIP). In FY17, the Division awarded three new YIP projects to drive fundamental research in areas relevant to the current and future Army. The following PIs and corresponding organizations were recipients of the new-start YIP awards.

- Professor Rahul Nandkishore, University of Colorado - Boulder; *Disorder and Interactions in Dirac Materials*
- Professor Chen Wang, University of Massachusetts - Amherst; *Non-reciprocal circuit quantum electrodynamics with ferrites*
- Professor Ilija Zeljkovic, Boston College; *Nanoscale Engineering of Superconducting Proximity Effect in Topological Insulator Thin Films*

4. Conferences, Workshops, and Symposia Support Program. The Division provided funds in support of a range of scientific conferences, workshops, and symposia that were held in FY17. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences, with the goal of supporting scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army, and to define the research needs, thrusts, opportunities, and innovation crucial to the future Army. Proposals requesting funding support, typically for less than $10K, were received and evaluated in line with the publicly available ARO BAA. In FY17, three proposals were selected for funding by the Division to support FY17 conferences, workshops, or symposia.

5. Special Programs. In FY17, the Division also awarded two new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school and undergraduate students. These efforts were funded through the ARO Core Program and Youth Sciences Programs, for research to be performed at academic laboratories currently supported through active SI awards (refer to CHAPTER 2, Section IX).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These projects constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Atomtronics: an Atom-Analog of Electronics. This MURI began in FY10 and was awarded to a team led by Professor Ian Spielman of the University of Maryland. The objective of this MURI is to explore and understand the concepts of atom-based physics, beginning with the rich and fundamental physics discoveries already revealed with cold atoms systems and to investigate the concepts required for future device applications.

Atom-based physics studies (atomtronics) are analogous to, but will go beyond, the fundamental twentieth century studies regarding the properties of electrons (*i.e.*, electronics) that enabled the electronics revolution. Solid-state electronics, heralded by the transistor, transformed both civilian and military culture within a generation. Yet there is only a single kind of electron: its mass, charge and spin (and thus quantum statistics as well) are unalterable. Atoms on the other hand, come with different masses, can have multiple charge states, and have a variety of spin and other internal quantum states. Accordingly, studies in atomtronics aim to understand an atom-based physics rather than electron-based device physics. Breakthroughs in cold atom physics and degenerate quantum gases presage this new kind of device physics. That cold atom science has resulted in atomic analogies to other technologies, such as optics and lasers, suggests that the same may be repeated with electronics. Very good analogies of solids and junctions can be made with trapped atoms. It is now well-known how one, two and three dimensional structures with essentially any lattice geometry can be formed in cold, trapped atoms. A few theory papers have pointed the way to simple devices.

The most apparent, but not necessarily the only approach to atomtronics, is through optical lattices, where Bloch's theorem holds. Band structure is the first basis on which physicists understand traditional (electronic) metal, insulator, and semiconductor behavior. Interaction and disorder modify this and exploration of Mott-like and Anderson-like insulators and transitions are envisioned as well. Doping can be mimicked by modifying atoms in certain wells or by locally modifying the lattice potential, which can be done with additional optical fields. Such defects could be deeper or shallower wells, or missing or additional sites. Recent breakthroughs involving three dimensional optical lattices and the loading of atoms into lattices with reasonably long lifetimes have set the stage for atomtronics.

Atomtronics researchers are focused on two key themes devices and connections. The envisioned analogs to devices can be described as those that perform actions under external control and those that can be cascaded. The researchers will explore spin-orbit coupling in atomic systems in an effort to exploit new degrees of freedom in "spintomic" device concepts as well as novel reversible logic via cascaded spintomic gates. In addition, researchers will investigate far from equilibrium regimes, which is not possible in condensed matter systems due to the residual phonon interactions at finite temperatures. The second theme centers on connections and is split between analogs to electronics and novel interfacing. The research team use the superfluid properties of ultracold atoms confined in rings to create circuits. These small circuits interact with lasers to demonstrate an analogous SQUID device. Finally the researchers are exploring novel interfacing by trapping atoms with evanescent waves along ultrathin optical fibers. It is hoped that this technique will allow several devices to be coupled while remaining isolated from the environment.

2. Multi-Qubit Enhanced Sensing and Metrology. This MURI began in FY11 and was awarded to a team led by Professor Paola Cappellaro at the Massachusetts Institute of Technology. The objective of this research is to explore and demonstrate imaging, sensing and metrology beyond the classical and standard quantum limits by exploiting entangled multi-qubit systems.

Precision measurements are among the most important applications of quantum physics. Concepts derived from quantum information science (QIS), such as quantum entanglement, have been explored for the past decade to enhance precision measurements in atomic systems with potential applications such as atomic clocks and inertial navigation sensors. QIS has also enabled the development of new types of controlled quantum systems for the realization of solid-state qubits. These systems could potentially be used as quantum measurement devices such as magnetic sensors with a unique combination of sensitivity and spatial resolution. However, progress towards real-world applications of such techniques is currently limited by the fragile nature of quantum superposition states and difficulties in preparation, control and readout of useful quantum states. The power of entangled and squeezed states for quantum sensing lies in their sensitivity to the external parameter to be measured.

This MURI aims to overcome three major obstacles to practical quantum sensor operation: the difficulty to experimentally create desired entangled many-qubit input states to the sensing device, the fragility of the states during signal acquisition, and low fidelity of the readout process. The results of this research may ultimately lead to dramatic improvements in imaging, sensing, and metrology.

3. Light Filamentation. This MURI began in FY11 and was awarded to a team led by Professor Martin Richardson at the University of Central Florida. The objective of this research is to establish the underlying qualitative and quantitative understanding of the physical phenomena associated with light filaments in order to create and control the filaments and their associated unique properties.

A light filament is a novel form of propagating energy that is a combination of a laser beam and plasma. A light filament has three characteristics that make it unlike any other form of energy, and also make it ideal for remote detection of trace materials. Like laser light, a light filament is coherent. However, unlike laser light, it undergoes wavelength dispersion as the beam propagates, creating a coherent beam with wavelengths across the entire visible spectrum. Since the beam contains laser radiation at every wavelength, it is sometimes called a super-continuum or white laser. The continuum has a high UV content, which makes it of interest for remote chemical spectroscopy. Finally, by beating the diffraction limit, a light filament does not diverge in space. Unlike any other form of energy propagation, a light filament can be as small at a distant target as it was when it was created. Light filaments are formed when intense laser pulses are focused down, due to the nonlinearity of the air (the Kerr effect), to about 100 microns. At this point, the intense field ionizes, creating a plasma. The plasma stops the self-focusing and equilibrium is reached. The complex interaction of the plasma and electromagnetic field creates these unique properties of light filaments. Although light filaments are extremely rich in phenomena for potential applications, the complex interaction of optical, plasma, and electromagnetic behaviors is poorly understood.

The research team is attempting to create light filaments and understand and predict light filament propagation characteristics, length, interactions with matter, and electromagnetic interactions. If successful, this research could ultimately lead to controllable light filaments that would revolutionize remote detection and imaging through clouds, creating a new ability in standoff spectroscopic detection.

4. Surface States with Interactions Mediated by Bulk Properties, Defects and Surface Chemistry. This MURI began in FY12 and was awarded to a team led by Professor Robert Cava at Princeton University. This project is exploring the recently-discovered class of materials known as topological insulators.

A topological insulator is a material that behaves as a bulk insulator with a surface that is metallic (permitting the movement of charges on its surface) due to the fundamental topology of the electronic band structure. This topological property separates it from nearly every other known phase of matter. Instead of a phase being due to a broken symmetry (such as results in crystalline, magnetic, superconducting, etc. phases), the property of metallic surfaces results from a transition between two topologically distinct phases: trivial and non-trivial. This is a parallel to the quantum Hall effect which also results from topology but it has two dramatic enhancements. First, it is not limited to two dimensions, and second, the physics should be able to survive to ambient conditions if materials are sufficiently clean. The quantum Hall effect and related phenomena require ultra-low temperatures and high magnetic fields to induce them. Topological insulators do not.

The objective of this research is to advance the discovery, growth, and fabrication of new bulk- and thin-film-based topologically-stabilized electronic states in which electron-electron interactions play a significant role. The researchers are bringing strong materials science, chemistry and surface science approaches to bear on the study of the novel properties of topological insulators. Research in this area has great potential for long-term benefits for the Army, such as electronically-controlled magnetic memory and low-power electronics.

5. High-Resolution Quantum Control of Chemical Reactions. This MURI began in FY12 and was awarded to a team led by Professor David DeMille at Yale University. This MURI is exploring the principles of ultracold molecular reaction, where chemical reactions take place in the sub-millikelvin temperature regime. This research is co-managed by the Chemical Sciences and Physics Divisions.

The study of ultracold molecular reactions, where chemical reactions take place in the sub-millikelvin temperature regime, has emerged as a new field in physics and chemistry. Nanokelvin chemical reactions are radically different than those that occur at "normal" temperatures. Chemical reactions in the ultracold regime can occur across relatively long intermolecular distances, and no longer follow the expected (Boltzmann) energy distribution. The reactions become heavily dependent on nuclear spin orientation, interaction strength, and correlations. These features make them a robust test bed for long-range interacting many-body systems, controlled reactions, and precision measurements.

The objectives of this MURI are to develop a fundamental understanding of the nature of molecular reactions in the nano-K temperature regime and to extend the cooling technique previously demonstrated by Professor DeMille[1] (through a previous ARO award) to other molecular candidates. The researchers are focused on the implementation of novel and efficient laser cooling techniques of diatomic molecules, and to understand the role of quantum effects, including the role of confined geometries, on molecules that possess vanishingly-small

[1] Shuman ES, Barry JF, DeMille D. (2010). Laser cooling of a diatomic molecule. *Nature*. 467:820–823.

amounts of thermal energy. This research could lead to new devices or methods that explicitly use quantum effects in chemistry, such as the precision synthesis of mesoscopic samples of novel compounds, new avenues for detection of trace molecules, and a new understanding of combustion and atmospheric chemical reactions.

6. Non-equilibrium many-body dynamics. This MURI began in FY13 and was awarded to a team led by Professor Cheng Chin at the University of Chicago. The goal of this MURI is to study fundamental non-equilibrium dynamics using cold atoms in optical lattices.

Dynamics far from equilibrium is of great importance in many scientific fields, including materials science, condensed-matter physics, nonlinear optics, chemistry, biology, and biochemistry. Non-equilibrium dynamics recently has taken on significance in atomic physics, where new tools will enable breakthroughs. In particular, optical lattice emulation is allowing one to gain insight, and potentially solve, traditionally intractable problems, including those out of equilibrium. Breakthroughs in other disciplines are also enabling a new look at non-equilibrium. In materials science, a recent pump-probe experiment enabled dynamical control of material properties.[2] Another example is in biochemistry, in determining the role that non-equilibrium phase transitions play in driven biochemical networks, e.g., canonical phosphorylation-dephosphorylation systems with feedback that exhibit bi-stability.[3-4] Despite the ubiquitous nature of non-equilibrium dynamics, little scientific progress has been made due to the many challenges, including the difficulty in finding many-body systems that remain far from equilibrium on experimentally accessible time scales.

The objective of this MURI project is to discover how many-body systems thermalize from non-equilibrium initial states, and explore the dynamics of far-from-equilibrium systems. Given that non-equilibrium dynamics plays an important role in many scientific and engineering areas, such as quantum sensing and metrology, atomtronics, and quantum chemistry, this research could ultimately lead to the development of dynamic materials, and devices for improved computation, precision measurement, and sensing.

7. Ultracold Molecular Ion Reactions. This MURI began in FY14 and was awarded to a team led by Professor Eric Hudson at the University of California - Los Angeles. The goal of this MURI is to design, create, and exploit molecular ion traps to explore precision chemical dynamics and enable the quantum control of ultracold chemical reactions. This research is co-managed by the Chemical Sciences Division.

Investments quantum computing and precision metrology have led to the development of molecular ion trap technology. These advances provide scientific opportunities that could be exploited to enable new methods for the study and control of chemical reactions. Recent scientific breakthroughs have been achieved in ultra-cold chemistry with neutrals, suggesting that ion chemistry would provide similar opportunities for an emerging new field. In addition, work in quantum information has led to the development of new types of arrayed micro-fabricated ion traps. Ion trap technology adds novel capabilities to molecular ion research, enabling new research opportunities in materials science, condensed-matter physics, chemistry, and biochemistry. In particular, ion traps offer dramatic improvements in chemical sensing at the single-ion level. Compared with molecular neutrals, trapped molecular ions offer interaction times much longer than what is possible in beam experiments; state preparation and readout is potentially cleaner; and Coulomb interactions with co-trapped atomic ions allow for general species-independent techniques.

The objective of this research is to develop and create molecular ion traps to exploit long interrogation time to study molecular ion chemistry, utilize extended interaction times and dipolar interactions in novel quantum control scenarios, improve chemical sensing using single-ion detection, and integrate the traps with various detectors. This research could ultimately leave to dramatically improved methods for creating and studying quantum dots, energetic compounds, biological reactions, and tools for detection of trace molecules.

8. Engineering Exotic States of Light with Superconducting Circuits. This MURI began in FY16 and was awarded to a team led by Professor Andrew Houck at Princeton University. The goal of this MURI is to initiate

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[2] Goulielmakis E, Yakovlev VS, Cavalieri AL, et al. (2007). Attosecond control and measurement: lightwave electronics. *Science*. 317:769-775.

[3] Qian H. (2006). Open-system nonequilibrium steady state: statistical thermodynamics, fluctuations, and chemical oscillations. *J. Phys. Chem. B*. 110:15063-15074.

[4] Ge H and Qian H. (2011). Non-equilibrium phase transition in mesoscopic biochemical systems: from stochastic to nonlinear dynamics and beyond. *J. R. Soc. Interface*. 8:107-116.

significant new experimental and theoretical explorations to harness recent breakthroughs in superconducting systems and to demonstrate useful new states of light that can be brought to bear on broader goals in sensing, measurement, simulation, and computation. This research is co-managed with the Electronics Division. If successful, this research may lead to new tools for metrology, could provide key insight into non-equilibrium quantum systems, and will provide new resources for quantum communication and sensing.

Quantum optics, particularly in the domain of cavity quantum electrodynamics, provides a pathway to create and use large macroscopic quantum states with photons. Such states have been difficult to generate because atoms trapped in a cavity provide only weak nonlinearity to mediate photon-photon interactions, high photon loss introduces decoherence, low photon collection and detection efficiency decrease success probability, among other challenges. On the other hand, recent progress in superconducting qubits and high-quality microwave cavities for quantum computing has enabled orders of magnitude improvements in coherence, fast single shot high-fidelity readout, high-fidelity quantum operations, low photon loss, and better understanding of decoherence mechanisms. These advances have enabled early experiments that have demonstrated the creation of high-fidelity coherent states with several tens of photons. In addition, the new generation of superconducting devices opens up the opportunity for the exploration of new regimes of quantum optics involving quantum states of 100s of photons. Further advances are possible if, in addition to the physics of quantum optics, advanced microwave circuit engineering is brought to bear on the regime of low-power microwave signals to improve coherence and function, and materials science is employed to determine relationships between decoherence and defects in materials, surface chemistry, and interface quality. In turn, the superconducting systems and the quantum states created in them could also be used as sensitive probes of materials behavior, in particular of the origin and sources of decoherence and dissipation mechanisms.

The multidisciplinary research team led by Professor Houck combines the efforts of physicists and engineers who will develop the theoretical and experimental tools to establish new regimes of quantum optics using superconducting circuits. The new states of light established in this program provide new tools for metrology, could provide key insight into non-equilibrium quantum systems, and in the long term may lead to applications in quantum communication and sensing.

9. Modular Quantum Systems. This MURI began in FY16 and was awarded to a team led by Professor Christopher Monroe at the University of Maryland – College Park. The goal of this research is to discover and explore modularity concepts for extensibility of small high-performance multi-qubit systems to larger systems with reduction of operational complexity. This research is co-managed by the Physics Division and AFOSR.

A paramount challenge in exploring physical systems (qubits) suitable for quantum information processing has been the contradictory requirement for precise manipulation of a quantum state on demand while maintaining strict isolation from the environment. Significant progress has been made in addressing this challenge. Coherence in several physical qubit types has improved by orders of magnitude. High fidelity fundamental quantum logic operations have been demonstrated. This progress has extended to multi-qubit systems involving a few (order ten) qubits. Progress continues to be made in improving coherence and fidelity. In parallel, advances have been made in connecting physically separated qubits. Key to these rapid advances has been a multi-disciplinary approach involving physics, materials science, control engineering, computer science, and mathematics, among other fields. A scientific challenge to further progress in the field has been the difficulty to add qubits and increase system size, while maintaining coherence and high-fidelity operations. System size needs to be increased before useful functionality can be explored and realized. Adding qubits increases the complexity of interactions between the qubits and makes layout, fabrication, and quantum control for high fidelity operations extremely challenging. Additional unwanted interactions introduce new qubit degrees of freedom to entangle with the environment and degrade coherence and fidelity. Modularity is a general scientific approach to address such complexity in which the system is decomposed into repeatable blocks with well-defined and controlled interfaces and interactions between the blocks and has been applied successfully to classical systems. Here, a module can be envisaged as a functional group of qubits and an interface. Exploring modularity for complex quantum systems is nascent but provides a potential extensible approach in which small numbers of high performance qubits can be extended to groups of high performance qubits and interfaces capable of precise manipulation within the group, between groups when required, and isolation from the environment and other groups.

Any quantum information processing system must balance the need for coherent control of the many interacting qubits necessary for a large-scale quantum system with decoherence rates that generally grow with system size. The objective of this research is to investigate a modular approach to constructing multi-qubit systems suitable for quantum information processing, to determine whether a modular system can achieve this balance and study the associated costs and benefits of taking the approach. In the long term, this research may overcome barriers and lead to new capabilities in the logistics, optimization, and the quantum simulation of materials.

10. **Discovering Hidden Phases with Electromagnetic Excitation.** This MURI began in FY16 and was awarded to a team led by Professor David Hsieh at the California Institute of Technology. The goal of this MURI is to discover and systematically explore hidden phases of materials induced with driven periodic excitation, to explore the unique physics and properties anticipated in those phases, and to illuminate the dynamics of the excitation process leading to them. This research is co-managed by the Physics (lead) and Materials Science Divisions.

Nascent research has demonstrated unique phases that are not adiabatically accessible from the known phase diagram. Recent discoveries have involved photo-excitation of a material with an ultra-short pulse which non-adiabatically induces a phase distinct from that existing elsewhere on the ground state phase diagram. Examples include a non-equilibrium superconducting state in a BCS superconductor, a ferromagnetic state in an antiferromagnetic oxide, and a unique metallic state in a thin film of a dichalcogenide. Also of interest are novel phases that can be adiabatically driven via a continuous periodic excitation (a.k.a. Floquet) that drives a material into a new phase (e.g. inducing a topological surface state in an ordinary insulator.) The additional time-periodic potential adds a new term to the Hamiltonian and drives, for example, transitions in orbital ordering, new electronic states with new crossings and avoided crossings, and resonant enhancement or reduction of superconducting order or charge and spin density waves.

Much opportunity is provided by recent advances in THz sources with MV/cm level electric fields which are sufficiently strong to provide resonant excitation of order parameters in strongly correlated materials. Additional opportunities are presented by van der Waals layered materials and free standing materials with reduced connections to the environment, thus limiting sources of decoherence. The objective of this research is to design, realize and manipulate new phases of matter using electromagnetic excitation that in the long term may lead to enhancements of electronic, optical, magnetic and thermal material properties that would lay a foundation for future technology in many areas.

11. **Abelian Bridge to Non-Abelian Anyons in Ultra-Cold Atoms and Graphene.** This MURI began in FY17 and was awarded to a team led by Professor Andrea Young at the University of California - Santa Barbara. The goal of this MURI is to unambiguously realize new systems exhibiting the physics of anyons and to verify their topological protection against decoherence.

The unparalleled potential capabilities of quantum sensors and quantum computers hinge upon finding systems that can be well controlled and robust against decoherence. Anyons are quasiparticles with fractional quantum statistics that can exist in low-dimensional systems and whose topological properties allow one to create quantum states that are protected from many sources of decoherence. The experimental evidence of the fractional quantum Hall effect (FQHE) was a landmark demonstration of topological order and fractional (anyonic) statistics in a two-dimensional electronic system. However, the fragility of the FQHE states, in which interesting anyons can exist, have prevented this approach from advancing despite decades of improvements in material quality. On the other hand, the recent experimental realization of Majorana modes by several groups provides an important scientific opportunity to explore these intriguing quasiparticles and provides a possible pathway to realize more general anyonic systems. Advances in 2D materials, including topological surface states, new measurement capabilities, and recent theoretical progress in analyzing strongly correlated systems are rapidly advancing toward additional breakthroughs. This MURI effort will include studies of intrinsic anyons alongside extrinsic, synthetic approaches. The realization of these new robust states can pave the way for advances in universal decoherence free quantum sensors and computation as well as provide materials with currently unachievable properties that can be explored scientifically.

C. Small Business Innovation Research (SBIR) – New Starts

The Division did not have any new-start SBIR contracts in FY17; however, the Division managed active projects continuing from prior years. A list of SBIR topics published in FY17 and a list of prior-year topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

The Division did not have any new-start STTR contracts in FY17; however, the Division managed active projects continuing from prior years. A list of STTR topics published in FY17 and a list of prior-year topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Serving Institutions (HBCU/MSI) – New Starts

The HBCU/MSI program encompasses the (i) Partnership in Research Transition (PIRT) Program awards, (ii) DoD Research and Educational Program (REP) awards for HBCU/MSI, and (iii) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY17, the Division managed three new REP awards, in addition to active projects continuing from prior years. In addition, proposals from HBCU/MSIs are often among the projects selected for funding by the Division (refer to the list of HBCU/MSI new starts in *CHAPTER 2, Section IX*.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The following PECASE recipient, previously nominated by this Division, was announced in this fiscal year by the White House. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

1. Novel Quantum Phases in Heavy d- and f-electron Systems Studied Using Nonlinear Optics. The objective of this PECASE, led by Professor David Hsieh at the California Institute of Technology, is to develop several non-linear optical (NLO) spectroscopies and microscopies that will enable the direct observation of multipolar order and to demonstrate the direct observation thereof in strongly correlated materials.

Multipolar order in heavy-electron materials may provide disruptive opportunities for the Army to maintain technological superiority on the future battlefield. Though no known technologies yet utilize multipolar electronic order, these phases may be suited for unforeseen advances in information processing and ultra-low power electronics. Such would advance the US Army's situational awareness and optimization of logistics, and provide new opportunities to reduce soldier burden via electronic technologies requiring significantly less electrical power.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY17, the Division managed six new DURIP projects, totaling $1.3 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. Joint Technology Office - High Energy Lasers (JTO-HEL)

The JTO-HEL program is funding MRI projects headed by Penn State and the University of Rochester to obtain high power lasers. The Penn State group uses a multiplexing system with timed laser pulses and a nonlinear optical element KTN (potassium tantalate niobate). The team is developing a series nanosecond timed laser pulses, all incident on the crystal at slightly different times. The heat properties of the KTN crystal are being studied, which will have an influence on the beam quality. A crucial limitation to high mode quality in fiber is TMI (thermal mode instability), a dynamic instability caused by high thermal loads. The Rochester group is solving this problem by developing index profiles that reduce modal instabilities. In particular, the group is developing fibers designed to have poor phase matching, reducing mode coupling, and therefore reducing TMI.

I. DARPA Quantum Assisted Sensing and Readout (QuASAR) Program

The goal of this program, co-managed by the Physics Division, is to bring state-of-the-art science of metrology and sensing and combine them with today's technological developments. The program goal is to bridge the gap between the best scientific performance and the appropriate packaging for fielding high-performance working sensors that are relevant to the DoD. This program was motivated in large part by the Physics Division and compliments ARO-supported research in ultracold gases, providing theoretical and experimental synergy to the Core program.

J. DARPA - Fundamental Limits of Photon Detection (Detect) Program

The Detect program seeks to establish the first-principles limit of photon detector performance. Currently, the performance of different classes of photon detectors varies significantly with respect to key metrics and fundamental limits of performance are not fully understood. Detect aims to establish these fundamental limits by developing new models for a variety of technology platforms and testing those models in proof-of-concept experiments. The program, co-managed by the Physics Division, is exploring whether new approaches could achieve the best performance characteristics from all current detection platforms and exceed current performance in all metrics simultaneously. The scope of this research effort is extremely well matched with efforts in the QIS program and work previously funded by ARO in single photon detection, a critical aspect of several quantum information processing approaches.

K. DARPA - Magnetic, Miniaturized, and Monolithically Integrated Circuits (M3IC) Program

The M3IC program is an initiative to enable the monolithic integration of magnetic materials with standard semiconductors for microwave circuitry that takes advantage of the functionality provided by the magnetic materials. Current state of the art utilizes bulky magnetic components that are separately manufactured and integrated further down the process chain. The M3IC program aims to eliminate this to enable much smaller and less costly radio frequency systems. The program is co-managed by the Physics Division and builds upon the physics of magnetic materials in the microwave frequency regime that was previously supported in the division.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Physics Division.

A. Novel Quantum Data Compression Algorithms for Quantum Simulation

Professor Alan Aspuru-Guzik, Harvard University, Single Investigator Award

The simulation of quantum systems was one of the first proposed applications of quantum computation in the early 1980s. Quantum simulators for quantum chemistry have since demonstrated the capability to efficiently calculate molecular energies for small systems and they have the potential to advance fields such as materials research, pharmaceutical drug design, and catalyst engineering. A limiting factor in realizing these capabilities, however, is the ability to successfully control the quantum resources required in the experimental simulation.

While many experimental groups are working to make harnessing these resources more tractable, in FY17 Professor Aspuru-Guzik and his team devised a novel quantum algorithmic strategy which instead reduces the resources required for quantum simulations. The group took inspiration from classical autoencoder networks, a type of learning neural network which forces data from large, input training data sets in high dimensions to lower, more tractable sets from which the original input can be recovered. This classical scheme is not practical to implement for quantum simulations because learning quantum encodings classically generally carries an exponential computational cost relative to the number of qubits in the simulation. The Aspuru-Guzik group followed a similar line of reasoning, however, to devise a novel "quantum autoencoder" capable of learning efficient encodings of quantum information. To illustrate the functionality of their approach, the Aspuru-Guzik group successfully demonstrated how an implementation of their quantum autoencoder learned how to compress the ground state wavefunction of a hydrogen molecule (see Figure 1). The results revealed a representative compression of the wavefunction of molecular hydrogen from four to two qubits, leveraging a training set of six ground states. The group's general model for a quantum autoencoder should, in turn, have applications outside of quantum simulation in areas such as compression protocols for quantum communication, error-correcting circuits, and quantum state preparation.

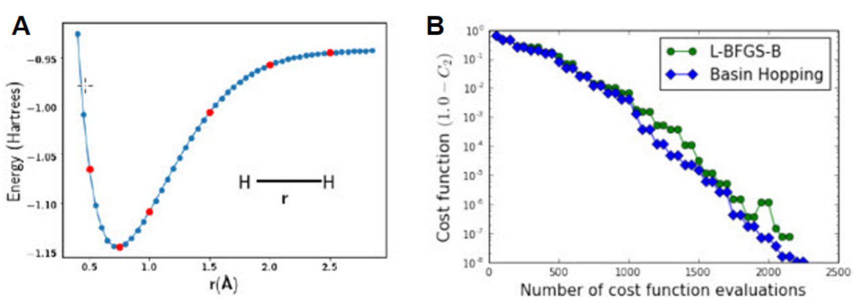

FIGURE 1

Compressing quantum data enables practical quantum simulations. (A) The exact potential energy surface for the hydrogen molecule is shown by the solid blue line. The red dots represent the training set of data for the autoencoder, and the ground states at the blue dots were used for testing. (B) The training process of the quantum autoencoder is shown by plotting the cost function as a function of the number of cost function evaluations for two different optimization algorithms employed in Aspuru-Guzik's approach. The data correspond to a compression of the wavefunction of molecular hydrogen from four to two qubits using a training set of six ground states.

B. Exploring Topological Physics with Light – Hofstadter Lattices in Qubit Compatible Cavity Arrays

Professor Andrew Houck, Princeton University, MURI Award

Improvements in superconducting quantum systems over the past decade have enabled their use in the exploration of entirely new regimes of physics, including the observation of topologically protected forms of light. In FY17, the MURI team lead by Professor Andrew Houck sought to leverage these advances to explore the possibility of constructing synthetic topological materials with microwave photons. While topological and strongly correlated material studies are at the forefront of research in condensed matter physics, it is experimentally extremely difficult to observe many of the properties of these systems in electronic materials, hence the Houck team's synthetic, light based approach. The work began with devising a scalable architecture for the exploration of interacting topological phases of photons in arrays of tunnel coupled, square microwave cavities. A key challenge in realizing this architecture is elucidating how to integrate non-reciprocal elements, which are required for breaking time-reversal symmetry and realizing the sought after topological physics. The Houck team overcame the obstacle by successfully coupling certain microwave cavities in the array to magnetic Yttrium-Iron-Garnet (YIG) spheres placed on three aluminum-post coaxial resonators in the center of the cavity (see FIGURE 2). The remaining lattice sites have single post coaxial resonators which oscillate in their fundamental mode with a spatially uniform phase profile. With these integrated attributes the lattice is fully capable of acting as a metamaterial which can realize topological physics.

The Houck team carried out a number of experiments to characterize the constructed synthetic topological insulator. To begin, they placed dipole antennas in each cavity to perform site-by-site spectroscopy with the aim of determining if the lattice displayed a defining characteristic of a topologically nontrivial band structure: insulating behavior in the bulk and conducting behavior along the edge. By probing the system edge within the energy gap of the bulk and measuring the phase accrued per lattice site as a function of frequency, the group was able to directly access the dispersion of the edge channel in their system. The team was further able to observe time-resolved edge-transport measurements which indicated that the applied pulses travel in one direction with a well-defined and constant velocity and exhibit no backscatter due to the protection provided by the chirality of the system. In total, the revealed insulating bulk and topologically protected chiral edge channels demonstrate that the group now has a toolbox for the development of low-loss topological microwave lattices. Moving forward, qubits will be integrated into the lattice to mediate photon-photon interactions and explore anionic physics and entanglement evolution in parametrically coupled edge channels. The platform is poised to provide the first exploration of strongly correlated topological quantum science in a synthetic system.

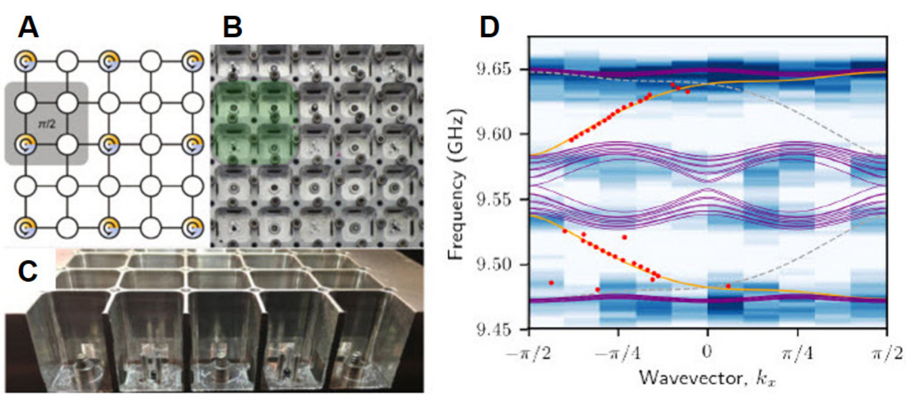

FIGURE 2

Exploring topologically protected states of light. The left side of the figure shows a schematic and photograph of the microwave topological insulator lattice. (**A**) Depiction of the cavity layout showing phase shifting YIG containing cavities (colored) and non-phase shifting cavities (white). This layout guarantees a phase acquisition of pi/2 per plaquette (gray). (**B**) A photograph of a 5x5 section of the lattice utilized in the experiment. (**C**) The side profile of the lattice shown in (B) where the three aluminum-post coaxial resonator cells which house the YIG spheres are clear. (**D**) The band structure of the quarter-flux Hofstadter lattice measured via site-by-site spectroscopy is shown. The bulk structure is represented by the blue/white density plot and the edge structure with the red points. For comparison, the theoretical predictions for a quarter flux Hofstadter strip are shown in purple/orange/gray-dashed and indicate excellent agreement with the observed data.

C. Optomechanics in Parity-Time Symmetric Photonic Structures

Professor Sahin K. Ozdemir, Pennsylvania State University, Single Investigator Award

This project relies on the synergy between the emerging fields of optomechanics and parity-time (PT) symmetric photonics. The objective is to precisely tailor photonic structures via tuning their coupling strength and loss-gain balance (or loss difference) to operate close to or away from non-Hermitian degeneracies known as exceptional points (EPs) for controlling light-matter interactions. Activities in the first year of this project resulted in multiple publications which investigate optomechanics and non-Hermiticity.[5-10] Of significant importance are the prediction[8] and the demonstration[9] of EP-enhanced sensing in cavity-assisted metrology, and the prediction of high-order EPs in optomechanics that helps to achieve higher cooling rates.[6]

Conventional sensing with optical cavities, nanoelectromechanical systems, and cavity-assisted metrology relies on the shift or splitting of a resonance frequency in response to a perturbation. These sensors are in general operated at a Hermitian degeneracy known as diabolic point (DP), and thus the amount of shift or splitting scales linearly with the perturbation strength. However, when they are operated at an *N*-th order EP, the shift or the splitting scales as the *N*-th root of the perturbation strength where *N* is the number of eigenvalues and eigenvectors of the system that coalesce at the EP (see FIGURE 3). Thus, a weak perturbation leads to a larger splitting when the system is operated at an EP. Loss-gain balance in a PT-symmetric system leads to narrower resonance linewidths or background spectra and helps to resolve the smallest amount of splitting or shift which could otherwise go undetected. The PI showed enhanced sensing at an EP, and confirmed that splitting scales as $\epsilon^{1/2}$ at a second order EP. For strong perturbations, sensors operating at a DP and EP performs similarly.

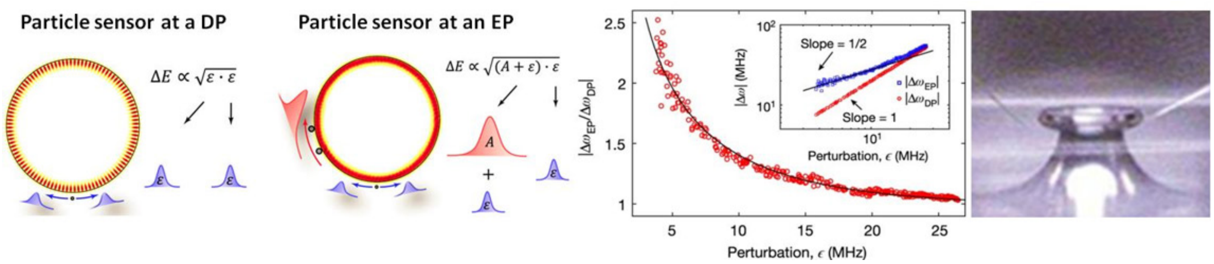

FIGURE 3

Electric-field distribution in a resonator operated at a DP exhibits standing waves. A target nanoscale object (small circle) scatters light in both clockwise- and anticlockwise-travelling directions (blue pulses), and leads to complex frequency splitting proportional to perturbation strength $\boldsymbol{\varepsilon}$. Electric-field distribution in a resonator operated at an EP exhibits travelling waves with a preferred direction due to intrinsic asymmetric backscattering (red pulse). This intrinsic backscattering together with the backscattering induced by the object results in complex frequency splitting proportional to $\boldsymbol{\varepsilon^{1/2}}$. Two grey circles represent the two scatterers used to tune the system to the EP. The ratio of mode splitting at an EP ($\Delta\Omega_{EP}$) to that at a DP ($\Delta\Omega_{DP}$) shows an enhancement for small perturbations. The sensor at DP exhibits a slope of 1, whereas the sensor at EP exhibits a slope of 1/2 (solid black line) for sufficiently small perturbations, confirming the square-root topology of EPs. A microtoroid resonator was also used, which was brought to a second-order EP by two nanoscatterers (silica nanotips) controllably-introduced into its mode volume. A third nanotip simulated the perturbation to be detected.

The presence of an EP enhances physical processes, interactions and system's response to perturbations. The higher is the degree of EP, the higher is the enhancement. High-order EPs were probed in purely optical systems. However, it was not clear how such high-order EPs can emerge in optomechanics and how they would affect optomechanical interactions. The PI showed the emergence of a third-order EP in a system of PT-symmetric resonators (see FIGURE 4). When this system is driven by an optical field red-detuned from the

[5] Asano M, et al. (2016). Observation of optomechanical coupling in a microbottle resonator. *Laser and Photonics Reviews* 10:603-611.
[6] Jing H, et al. (2017). High-order exceptional points in optomechanics. *Scientific Reports* 7:3386.
[7] Liu YL, et al. (2017). Controllable optical response by modifying the gain and loss of a mechanical resonator and cavity mode in an optomechanical system. *Physical Review A* 95, 013843.
[8] Liu ZP, et al. (2016). Metrology with PT-symmetric cavities: Enhanced sensitivity near the PT-phase transition. *Physical Review Letters* 117:110802.
[9] Chen W, et al. (2017). Exceptional points enhance sensing in an optical microcavity. *Nature* 548:192.
[10] Asano M, et al. (2016). Anomalous time delays and quantum weak measurements in optical microresonators. *Nature Communications* 7:13488.

resonance with a detuning larger or smaller than the mechanical frequency, only a second-order EP emerges. However, when the red-detuning matches the frequency of the mechanical mode, the supermode structure radically changes, featuring a third-order EP. This third-order EP enhances both the mechanical damping and the spring stiffness, which in turn facilitates low-power phonon (mechanical) cooling, with improved rates beyond what is achievable in conventional cavity optomechanics. In contrast to conventional systems, in an EP-assisted cooling scheme both the optical spring and the mechanical damping play significant roles leading to more than two-orders of magnitude improvement in cooling rates. These findings provide new insights for low-power optomechanical and phononic devices.

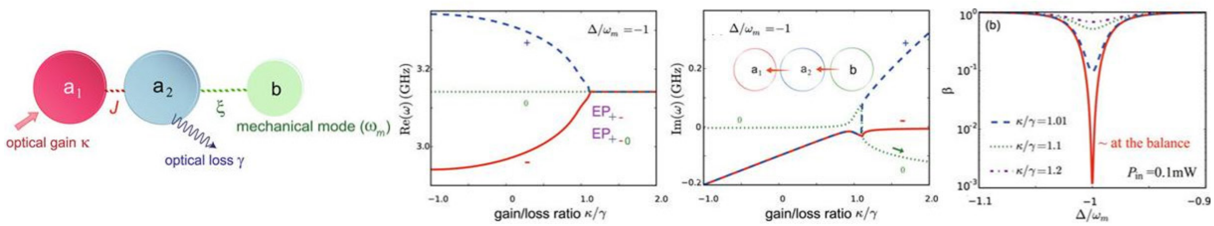

FIGURE 4

Model of an optomechanical system composed of PT-symmetric microresonators. For a red-detuned drive (Δ/ω_m=-1), supermodes of the system coalesce at an EP creating third-order EP. This modifies the energy flow in the system such that energy of the mechanical mode is transferred to the optical modes. As a result, when the system is at exact loss-gain balance and the drive is red-detuned the enhancement in the cooling rate as defined by the inverse of $\beta = n/n_o$ (ratio of the phonon number n in the PT-symmetric system at third-order EP to the phonon number n_o in a conventional optomechanical system) reaches as high as thousand at the drive power of 0.1mW. This cooling rate is at 0.1 mW is two orders of magnitude higher than that of a conventional system driven at P_{in} = 1 mW, implying a significant benefit in terms of power budget for cooling.

D. A New Platform for Fractional Quantum Hall Physics

Professor Andrea Young, University of California Santa Barbara, Single Investigator Award

The fractional quantum Hall (FQH) effect discovered in the 1980s was formerly considered a potential platform for quantum computing due to the non-Abelian quantum statistics of quasiparticles anticipated to be present. However, it was discarded for this potential application roughly a decade ago due to the extremely fragile nature of the FQH states proposed for this purpose. A new materials system, encapsulated bilayer graphene, may now re-energize such possibilities.

The integer quantum Hall effect occurs in high quality two dimensional electron systems in the presence of a perpendicular magnetic field. It can be understood semi-classically as the result of electrons bouncing around the edges of the sample, while bulk electrons circulate in tight, immobile orbits and are left out of the action at the edges. For certain ranges of magnetic fields, the edge conduction is quantized to a specific multiple of the conductance quantum, e^2/h, where e is the fundamental charge and h is Planck's constant, providing the metrological definition of the Ohm, the standard unit of electrical resistance. Between these 'magic' magnetic fields, even more interesting physics arises in the highest quality samples: the FQH effect. Here, states similar to the integer quantum Hall effect arise but with rational fractional values. Many FQH states are well described as arising from the motion of new composite particles consisting of electrons bound to two or more magnetic flux lines. Within FQH states, additional energy can be added to the system in the form of 'fractionalized' particles, carrying a charge that is some fraction of e. Remarkably, some of these fractional states are expected to host new particles whose very quantum statistics are fractionalized. This behavior is fundamentally different than all other known matter which is either bosonic (for example, photons) or fermionic (for example, electrons). The FQH effect has been observed in AlGaAs/GaAs quantum wells for several decades and has been studied extensively. However, the states are extremely fragile and not only are rather heroic experiments necessary to study the state, samples of sufficient quality to observe them are available from only a few sources.

Graphene is a naturally two dimensional electron system and the quantum Hall effect was observed in this material not many years after its discovery. The most notable advances in quantum Hall physics in graphene have not been so much due to the improvement of the graphene itself but in the handling and packaging of the graphene. Physical wrinkles, charge impurities and variations in the dielectric constant of surrounding materials on the scale of the mean free path of electrons in graphene result in a very rough energy landscape through which those electrons must travel. Sandwiching graphene between sheets of hexagonal boron nitride (hBN) smooths out wrinkles and minimizes charge impurities, both of which are of major concerns in SiO_2 which was formerly the material of choice on which to place graphene. Professor Young and his team further employed graphitic gates (instead of traditional metallic gates) on both the top and bottom of an hBN/bilayer graphene/hBN sandwich to further smooth out the energy landscape. The result was remarkable; in both GaAs and former studies of the FQH effect in graphene, a magnetic field of several Tesla and exceptionally low temperatures—usually below 100 millidegrees—were necessary to observe the effect (see FIGURE 5). In these samples, the FQH states became evident at several times higher temperature at magnetic fields as low as 1 Tesla. The magnetic field used in this experiment was 14 Tesla where the fractional states are easily observed. A large capacitance (yellow in the color plot) reveals the presence of either an integer or fractional quantum Hall state. This capacitance measures the energy necessary to inject an electron into the state and is a direct measure of the robustness of the state. For the most exotic states, thought to host exotic nonabelian quantum statistics, this energy gap was found to be roughly quadruple that of equivalent states in the AlGaAs/GaAs system. This is particularly remarkable since graphene was discovered only 13 years ago whereas the GaAs system has been studied for many decades.

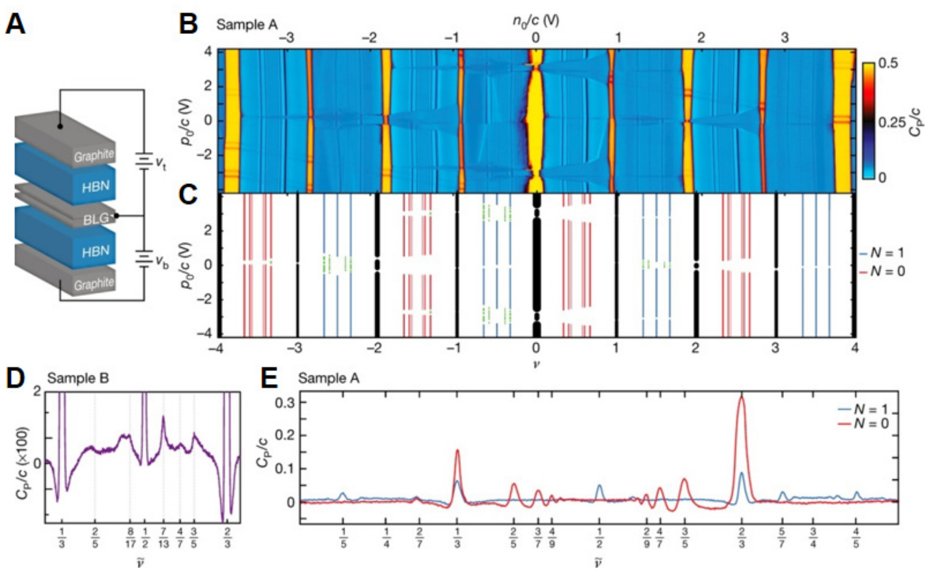

FIGURE 5

Integer and Fractional quantum Hall states of bilayer graphene. (**A**) Schematic of the bilayer graphene sample. (**B**) Capacitance data and (**C**) a representation thereof for the bilayer system as a function of the voltage on the two sides of the sample. (**D**) A detailed view of the capacitance showing the detail of several important fractional states. (**E**) The capacitance of fractional states between zero and one for one sample.

The stability of the FQH states in encapsulated bilayer graphene is noteworthy and provides a unique opportunity to study details associated with these novel topological states. While heroic experiments in GaAs continue to provide steady advances in the insight of fractional states, graphene is far more accessible. Instead of painstaking molecular beam epitaxy and sample preparation, encapsulation of graphene is done by hand with merely an optical microscope. While low temperatures and high magnetic fields are still necessary, the greater availability of suitable samples will accelerate this field dramatically in the years ahead. Furthermore, as the states are much less fragile, it may invigorate another look into the potential of using the FQH states for quantum information processing.

E. Collective Emission of Matter-Wave Jets from Driven Bose-Einstein Condensates

Professor Cheng Chin, University of Chicago, MURI/Single Investigator Award

Many important physical phenomena depend on whether spontaneous or stimulated scattering dominates. Spontaneous will often dominate when the scattering rate is low. When the scattering rate is increased passed a certain threshold, stimulated emission can dominate, leading to an exponential amplification. This can result in a markedly different behavior. For example, the laser upon achieving a sufficient rate of stimulated emission will produce coherent light. ARO funded researchers at the University of Chicago have shown that runaway stimulation of collective atom–atom scattering in a driven Bose-Einstein condensate will result in the amplification of matter-wave jets.

The experiment consisted of trapping approximately 30,000 cesium atoms in a pancake-shaped optical trap (see FIGURE 6).[11] The atoms were cooled to form a Bose-Einstein condensate that is tightly confined in the z-direction. The depth of the trap was sufficient to confine the condensate in all directions, but weak enough to allow for ejected atoms to propagate.

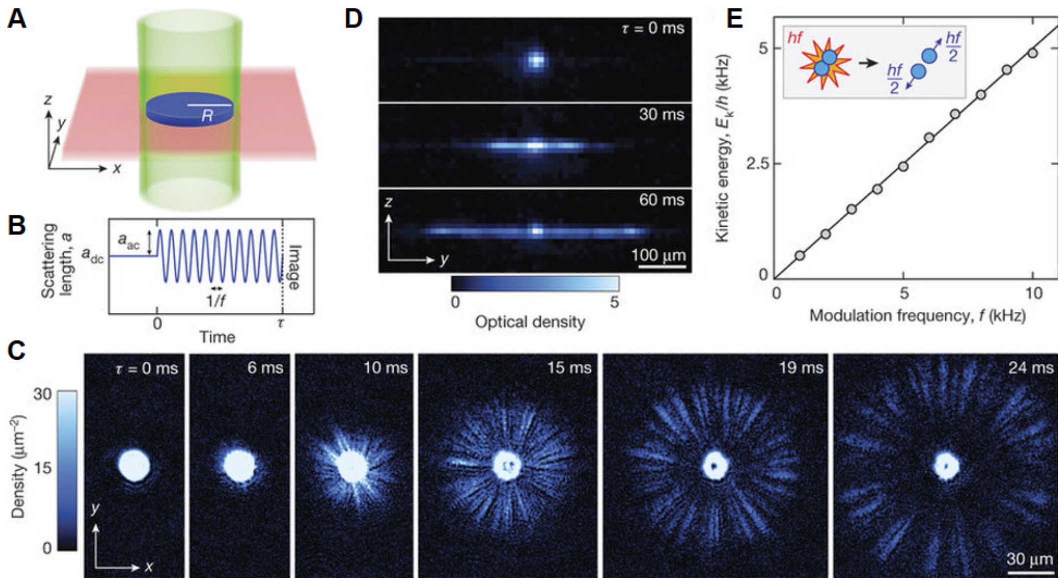

FIGURE 6

Two-dimensional emission of matter-wave jets from Bose–Einstein condensates with modulated interactions. (A) Disk-shaped Bose–Einstein condensates (blue) of radius R are trapped at the intersection of two lasers, which create a repulsive cylindrical shell (green) and an attractive sheet (red). (B) In a typical experiment, we modulate the scattering length as $a(t) = a_{dc} + a_{ac}\sin(\omega t)$, where $\omega \equiv 2\pi f$, for a time τ before collecting an image of the resulting density distribution. (C) Top-down images of condensates obtained after modulating the scattering length at $f = 3.5$ kHz and $a_{ac} = 60a_0$ show condensates ejecting a sudden burst of narrow jets. Note that the internal structure of the remaining condensate suffers from imaging artefacts owing to the extremely high density of the condensate. (D) Side-view images of the condensates taken at $f = 3.5$ kHz show atoms emitted predominantly in the horizontal plane. Each image in C and D corresponds to a single, independent realization of the experiment. (E) Measured mean kinetic energy per emitted atom for a range of modulation frequencies. The standard error of the mean is smaller than the symbol size. The solid line shows the expected kinetic energy $E_k = hf/2$. The inset illustrates the microscopic process leading to jets: two atoms collide, absorb one energy quantum from the oscillating field and are ejected in opposite directions.[11]

Once the condensate was loaded into the trap, the magnetic field was modulated near a Feshbach resonance, which resulted in the s-wave scattering length of the atoms to oscillate. A typical experiment consisted of maintaining a small, positive scattering length $a_{dc} = 5a_0$, where a_0 is the Bohr radius, the modulation amplitude was held at a constant value a_{ac} for a duration τ before imaging the atomic density distribution. During the first few milliseconds of the modulation there was very little observable change. However, once a threshold was achieved the jets suddenly emerged and propagated radially outward form the condensate. Each repetition of the experiment appeared to result in a random pattern. However, the jets that formed all had similar angular widths and were often accompanied by a counter propagating partner. This behavior was consistent for a range of frequencies $f = 1$–10 kHz and were predominantly ejected in the horizontal plane. To model this process, the kinetic energy per atom was determined by tracking the distance the atoms travel over time. It was estimated that each atom had on average a kinetic energy equal to half a quantum of the oscillating field, $E_k = hf/2$, where h is the Planck constant.

[11] Clark LW, Gaj A, Feng L, Chin C. (2017). Collective emission of matter-wave jets from driven Bose-Einstein condensates. *Nature*. 551:356-359.

To understand the microscopic process responsible for the ejection of atoms, the kinetic energy per atom was extracted by monitoring the distance of the atoms from the condensate over time. It was determined that each atom had kinetic energy equal to half of the quantum of the oscillating field. This would indicate that the ejected atoms result from collisions in which two atoms absorb and equally share an energy of hf from the modulation and are ejected in opposite directions, during which counter-propagating pairs of atoms are ejected while conserving momentum and energy.

The presence of preferential emission in the horizontal plane and the structure of the jets indicate a collective collision process, which occurs throughout the condensate. If the s-wave collisions were uncorrelated they would produce a diffuse, spherical shell of outgoing atoms. The features observed in this experiment suggest each collision stimulate further scattering into the same outgoing direction. In the presence of sufficient driving the stimulated emission results in a large number of atoms appearing as jets and suppressing emission in other directions.

ARO funded researchers at the University of Chicago have studied the structure and occupation of jets that stem from quantum fluctuations of a Bose-Einstein condensate. The results indicate that the firework patterns observed in the emission emerge from quantum fluctuations. These results further the investigations in non-equilibrium many-body physics which underpins our understanding in material design and the microscopic dynamics of quantum systems.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Monolithic Integration of Magnetic Materials for On-Chip Non-Reciprocal Function

Investigator: Professor Z. Celinski, University of Colorado - Colorado Springs, MURI and Single Investigator Awards
Recipient: DARPA

From 2000-2015, Professor Celinski and his colleagues studied magnetic materials for on-chip microwave frequency functionality with ARO support. The effort included both theoretical and experimental studies. The theoretical initiative provided the foundational basis for the linear and non-linear magnetic response of thin films and nano- and micro-structured magnetic materials transporting and modulating spin waves at microwave frequencies. Guided by these studies, experimental efforts focused on measurements of the high frequency response of microwave waveguides incorporating a variety of magnetic materials (both metallic such as permalloy and insulating such as yttrium iron garnet) and correlating the response with the material quality, microstructure and interfaces, and device geometry. The result of this initiative was a body of work detailing how thin magnetic films, patterning and device geometries could be utilized to manipulate spin waves in the range of 10 – 60 GHz. Technologically, the value of magnetic materials is that they can provide non-reciprocal function – different behavior for spin waves flowing in opposite directions – without the need for an external magnetic field or bias magnet.

These results transitioned in FY17 to form a key basis for a relatively new DARPA program entitled Magnetic Miniaturized and Monolithically Integrated Circuits (M^3IC). The goal of this program is to utilize magnetic materials such as those explored in the single investigator and MURI efforts for monolithic integration with traditional microwave materials. The DARPA program began in FY17 and is a multi-year effort involving both grants to universities and contracts to demonstrate unique non-reciprocal functionality provided by magnetic materials in a miniaturized form as was revealed to be possible by the ARO-supported efforts.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Exploring Silicon Vacancy Centers in Diamond for Quantum Information Implementations

Professor Jelena Vuckovic, Stanford University, Single Investigator Award

Silicon-Vacancy (SiV) color centers in diamond have recently demonstrated excellent spintronic and optical properties, making them promising candidates for scalable quantum information processing architectures. One primary challenge currently inhibiting the full exploitation SiVs is that they have relatively short coherence times, which, in turn, makes it relatively difficult to carry out useful numbers of operations on them.

In FY18 Professor Vuckovic will explore ways to combat these short coherence times as part of a new single investigator award. A primary source of decoherence in SiV systems comes from the centers' two nondegenerate orbital ground states readily coupling to phonons in the diamond, and research during the first year of the project will explore possibilities for suppressing the phonon density of states near the 50 GHz coupling frequency. One promising pathway for this is to embed single SiV centers in specially designed nanostructures. Specifically, the team will design and optimize nanostructures with footprints which force boundary conditions on phonon vibrations and consequently lead to phonon suppression below 50 GHz. This approach effectively removes the source of decoherence. Additionally, the team will work to maximize the number of operations possible on the SiV centers before they decohere by devising optical pulse sequences which initialize, coherently rotate, and readout single SiV spins. This should enable a dramatic increase in the number of qubit interactions one can implement before coherence is lost. It is anticipated that the combined results of these two approaches will ultimately aid in making SiV centers attractive candidates for qubit based systems.

B. Controlled Release of Energy from Nuclear Isomers by Laser-Driven X-Rays

Professor Donald Umstadter, University of Nebraska, Single Investigator Award

The objective of this research is to discover energy-release channels for several nuclear isomers, making it possible to identify isomers that are viable for high-density energy storage and controlled release through optical means. Professor Don Umstadter of the University of Nebraska, working with researchers at ARL-SEDD, have successfully performed the first isomer-population experiments on 115-In using Nebraska's laser-based source. This was accomplished using bremsstrahlung and broad Thompson scattering beams, and presently the team is finalizing the analysis of the results, which indicate production of other short-lived (minutes to hours) radioactive species, including gamma rays and fast neutron induced reactions. It is anticipated that in FY18, the team will perform a complete narrow Thompson beam scan over the known isomer-population resonances of 115-In to demonstrate the utility of this technique for nuclear studies, including for later tests of isomer depletion (with energy release) for other nuclides. With these results, the most suitable isomer for energy sources will be identified.

C. Terahertz-Modification of Graphene

Professor Junichiro Kono, Rice University, Single Investigator Award

Recent studies on the interaction of electromagnetic radiation with matter have revealed the potential to fundamentally alter the electronic, magnetic and optical properties of those materials both during the presence of the radiation and as a long-lived metastable state after the radiation has subsided. Because coherent radiation induces a time-oscillating potential energy profile, it is described by a differential equation akin to the Schrödinger equation that describes the electronic energy states in a crystal – a physically periodic potential energy profile. Time-oscillating potential energy profiles can give rise to distinct energy states for electrons. These are referred to as Floquet phases or states. The availability of high-intensity THz sources is in many ways enabling the study of Floquet states in electronic materials. THz radiation is low enough in energy that it does not damage materials physically, yet it provides a meaningful coherent interaction for materials. Graphene is a particularly useful material in which to explore these interactions and the possibility for new phases. Graphene is readily prepared with extremely high quality so that defect-dominated effects do not hide the physics of interest. It is a single atom thick so that the entire irradiated material experiences the same electromagnetic field. Furthermore, there have been a variety of theoretical predictions of how the electronic properties of graphene are fundamentally modified by electromagnetic radiation. Examples include inducing carrier population inversion (such as is employed for lasing), extreme non-linear optical properties and topologically non-trivial states.

It is anticipated that in FY18, Professor Kono will explore these possibilities experimentally to determine how challenging these theoretical proposals are to achieve. If successful, this research may enable new approaches to optoelectronic devices and nonlinear optical elements in a low-cost material system for a plethora of Army applications.

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